Geometric Rigidity and an Application to Statistical Mechanics

by

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Declarations

I declare that this thesis has been written solely by myself. Its contents have not been submitted previously in application for a degree. The work done in this document was performed by myself. I was provided guidance on its subject matter by my PhD supervisor Dr. F. Theil. In the case where work is based on previous results by others this is explicitly stated in the text.

Abstract

In this thesis we generalise the rigidity estimates of Friesecke et al. [2002] and Müller et al. [2014] to vector fields whose properties are constrained by both conditions on the support of their curl and the underlying discrete symmetries of the lattice $\mathbb{Z}^2$. These analytical estimates and other considerations are applied to a statistical model of a crystal containing defects based on work by Aumann [2015]. It is demonstrated in this thesis that we allow a finite density of defects. The main result is that regardless of crystal size, the *ordering* of the crystal, expressed via the L^2-distance of a random vector field from the rotations, can be made arbitrarily small for sufficiently low temperature β^{-1}.

Chapter 1

Introduction

1.1 Ordering and Statistical Mechanics

The contents of this thesis are concerned with providing a series of generalisations to a rigidity estimate originally proved in Friesecke et al. [2002], with a view to applying this estimate to a statistical model of a crystal at finite temperature. The main idea of this estimate is that expresses the *ordering* of a system of points in a particular sense. Research into systems in which some kind of ordering occurs at low temperature systems is extensive. Reviews of classical examples of other kinds of ordering can be found for instance in Bhattacharjee and Khare [1995], and Kosterlitz [2016]. We will briefly discuss a model of a crystal introduced in Heydenreich et al. [2014], based on a model of Merkl and Rolles [2009], to motivate this discussion. In Heydenreich et al. [2014] the orientational ordering of a model of a two-dimensional crystal at finite temperature is considered, where the crystal may have some small defects. The domain the crystal lives in, U_n, is taken to be an appropriate affine transform of $n[0,1]^2$ and is equipped with periodic boundary conditions. Atoms are indexed by their sites on a truncated triangular lattice $\Lambda_n = \Lambda \cap U_n$. Here Λ denotes the triangular lattice, given by

$$\Lambda = \frac{1}{2}\begin{pmatrix} 2 & 1 \\ 0 & \sqrt{3} \end{pmatrix} \mathbb{Z}^2.$$

In Heydenreich et al. [2014] atoms either have a position in space, or can be denoted as missing- a *defect* known as a vacancy. A *displacement field* u^ω is defined through a piecewise affine interpolation of the atomistic displacements. Where an atom is absent, the average position of its neighbours is taken to establish the periodic vector field $u^\omega(x)$ defined on the box U_n. Note that in the above, an *extension* of u^ω into the defects was used, an important step as will be discussed later. The energy of configuration $\omega = \{\omega(x), x \in \Lambda \cap U_n\}$, and $\omega(x) \in \mathbb{R}^2 \cup \circ$, is given by

$$H(\omega) = \sum_{x \in U_n \cap \Lambda} \left(\sum_{y \sim x} \chi[\omega(x), \omega(y) \in \mathbb{R}^2] \cdot V(|\omega(x) - \omega(y)|) + \sigma \chi[\omega(x) = \circ] \right),$$

with $V(1) = 0$, and $V'' > 0$ near 1. In the above two lattice sites x, y are connected if they are nearest neighbours in the triangular lattice. This is denoted $x \sim y$. The indicator function $\chi[\cdot]$ equals 1 if the expression in the square brackets is true, and 0 otherwise.

The set of all configurations are restricted to the set Ω_n, which contains only configurations with "small" maximum strains. That is, $|u^\omega(x) - u^\omega(y) - (x-y)| < \varepsilon$ for $x \sim y$, with ε a sufficiently small given model parameter. The second term in the energy punishes the number of vacancies in the crystal, where σ determines the strength of this punishment. A probability measure

$$P_{\sigma,\beta,n}(d\omega) = Z^{-1}_{\sigma,\beta,n} e^{-\beta H(\omega)} \mu_n(d\omega), \quad Z_{\sigma,\beta,n} = \int_{\Omega_n} e^{-\beta H(\omega)} d\mu_n$$

where μ_n is the reference measure $(\lambda_2 + \delta_\circ)^{\Lambda \cap U_n}$, where λ_2 is the two-dimensional Lebesgue measure and $\delta_\circ(\omega(x)) = 1$ if $\omega(x) = \circ$ and 0 otherwise. Defining the *tiling* T_n consisting of the triangles t upon which $\nabla\omega$ is constant on, and under some other technical assumptions, the result

$$\lim_{\beta \to \infty} \limsup_{n \to \infty} \sup_{t \in T_n} \mathbb{E}_{\sigma,\beta,n}[|\nabla u^\omega(t) - I|^2] = \lim_{\beta \to \infty} \limsup_{n \to \infty} |T_n|^{-1} \mathbb{E}_{\sigma,\beta,n} \|\nabla u^\omega - I\|^2_{L^2(U_n)} = 0. \tag{1.1}$$

As discussed in Heydenreich et al. [2014] while the underlying energy is rotationally invariant, states themselves are not in the large β limit. The displacement map u^ω encodes how ordered each configuration is, and its statistical properties are what are used to discuss ordering. Particular to low dimensional systems, however, this does not imply statements about the expectation $\mathbb{E}_{\sigma,\beta,n}[|u^\omega(0) - u^\omega(x)|^2]$ for large x. This quantity represents *translational* ordering. While of great interest in its own right (See for instance Richthammer [2007], Fröhlich and Pfister [1981], Mermin [1968]) it is not considered in this thesis.

1.2 Defects, Symmetry & Defining Order

Implicit in the demonstration of (1.1) for a lattice model are statements on the existence of an object measuring a configuration's *orientational ordering*, along with this object's (and its extension's) regularity in the presence of defects. The above mappings u^ω are global objects with enough regularity to avoid dealing with the discrete properties of Λ. To generalise the above to other statistical models (containing more complex defects) we must make analytical statements about vector fields defined on a continuum domain U_n whose properties encode the behaviour of a given discrete symmetry group.

In this section we establish what we mean by the concept of orientational ordering for more general vector fields of varying regularity. For simplicity we will now work with a square lattice, $\Lambda = \mathbb{Z}^2$. While there is a rich literature devoted to understanding this and similar topics (Kleinert [2008] is a comprehensive introduction), as mathematical analysts we have decided to work on a specific formulation of this problem that is more limited in scope, and is amenable to study by analytical methods. We now consider portions of the lattice $\mathbb{Z}^2$ that have been made defective in some way, and what problems this presents when quantifying their disorder.

1.2.1 Translational Symmetry & Ordering

Consider the configuration below, where we consider the set of all unshaded deformed squares as constituting a tiling T^ω of the set of points $\omega = v(T^\omega)$, the vertices of all tiles.

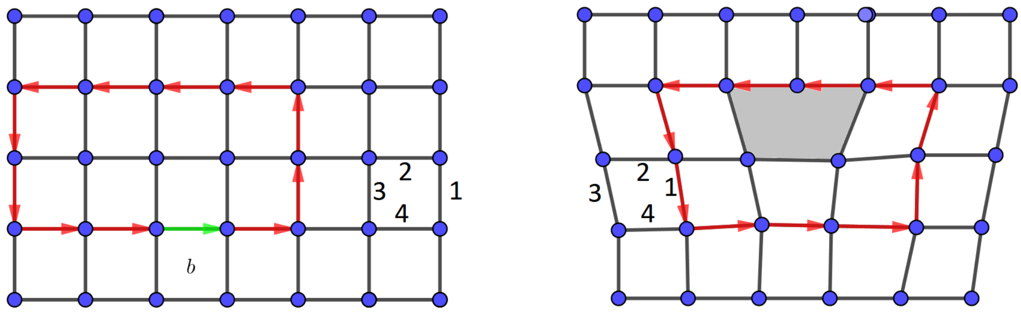


Figure 1.1: A dislocation. We have chosen a tile above and labelled its edges 1,2,3,4 in an anti-clockwise fashion. There are more horizontal (even-numbered) edges above the shaded region than below, as making a circuit with the same number of steps in both configurations demonstrates.

This kind of defect is known as a dislocation (Hull and Bacon [2011]). Intuitively (to begin with) we must decide what part of the configuration is at least *locally* "like a lattice" and which is not, in this case the unshaded and shaded part of the figure respectively. Note that as the figure shows there is now no global bijection from ω to $\Lambda\backslash\overline{B}_1(0)$. This is due to the extra half-line of atoms that has been inserted into the configuration on the right. It is for this reason we emphasise that ω can at most be locally lattice-like. We now discuss how to quantify this idea. As before we wish to define some piecewise affine interpolant of the positions of atoms on the region $\cup_t T^\omega$. There is no continuous $u^\omega : \cup_t T^\omega \to \mathbb{R}^2$ (in fact the inverse of the mapping used in (1.1)) such that $u^\omega(x) \in \Lambda$ for each $x \in \omega$[1]. We will instead analyse this configuration using a covering and local displacement maps, before finding a *global* means to describe the configuration later. We first choose a sense in which we will map each tile in the tiling T^ω to ones in the reference lattice. This is where the rotational symmetry group of the lattice first makes an appearance. Define

$$\Gamma(\mathbb{Z}^2) = \{\gamma \in \mathrm{SO}(2) : \gamma\mathbb{Z}^2 = \mathbb{Z}^2\}.$$

As shown in Figure 1.1, where we labelled tile edges, we will always choose a displacement map that takes the rightmost edge of a tile in T^ω to the rightmost edge of a tile in $T^{\mathbb{Z}^2}$. We can describe this by propagating the labelling of edges on the tile in the left and right side of the figure to the other tiles therein. That is, for any local displacement, we map edges in a way that preserves orientations: we will never map an edge labelled '1' to one labelled '2'.

The underlying assumption that should not be made is that this is possible for all locally lattice-like configurations, which will be discussed in the next subsection. At least for this configuration one of four *consistent* labellings can arbitrarily be chosen. Once this is decided we take a covering $\{S_i\}_{i=1}^J$ of T^ω comprised of overlapping, simply connected sets. On any such set we have a choice of any mapping

$$u_i(x) + \lambda, \lambda \in \Lambda,\ x \in \bigcup_{t \in S_i} t := \cup_t S_i,$$

that map $\cup_t S_i$ to a region in $\mathbb{R}^2$ and $u_i(\omega \cap S_i) \subset \Lambda$. Making choices $\{\lambda_i\}$ in the above, and provided the same edge labelling scheme was used on each S_i different maps satisfy the relation

$$u_i - u_{i+1} = \tilde{\lambda}_i \in \Lambda$$

[1] This is discussed in detail in Chapter 3.

on $S_i \cap S_{i+1}$. As discussed above, there is no way to choose the set of $\tilde{\lambda}_i = 0$ for all i, stopping us from defining a global continuous displacement map. It is also evident that such a construction to describe a crystal locally is unwieldy. To get around this, we can instead look for a way to work with a vector field defined on all of $\cup_t T^\omega$ that is locally a gradient. Locally we would then recover the above picture, but we would have a single, globally defined object that only involves a single choice of orientation. This idea follows from a generalisation of work done in Aumann [2015]. We can define a vector field V^ω as follows:

$$V^\omega : \cup T^\omega \to \mathbb{R}^{2\times 2} : \quad V^\omega(x) = \nabla u_i^\omega(x), \ x \in S_i \tag{1.2}$$

where since the displacement maps differ by a constant, the above is well defined. We receive a vector field V^ω such that $\operatorname{curl} V^\omega = 0$ on $\cup T^\omega$, but (as V^ω is defined through the gradient of displacements)

$$\oint_{\text{red circuit}} V^\omega \cdot dl \in \Lambda.$$

and so (after an edge labelling) we receive a globally defined V^ω that encodes a way to detect the kind and location of defects present in ω. It can be seen by inspection there is a surplus of one kind of edge around the dislocation co-inciding with the circulation. For this and other similar vector fields, we consider the following problem:

Order In The Presence of Translational Defects

Let $D^\omega = U_n \backslash T^\omega$ denote some small, isolated regions $D_1^\omega, D_2^\omega, \ldots$. Then for

$$V^\omega : \operatorname{curl} V^\omega = 0 \text{ on } \cup T^\omega, \ \oint_{\partial D_i^\omega} V \cdot dl \in \Lambda,$$

$$\text{estimate } \min_R \|\gamma_T V^\omega - R\|_{L^2(\cup T^\omega)}, \text{ where } \gamma_T \in \Gamma(\mathbb{Z}^2), \ R \in \mathrm{SO}(2). \tag{1.3}$$

The global choice γ_T from the lattice's discrete symmetry group is arbitrary. While we cannot work directly with the gradient of a global displacement due to the translational symmetry of the lattice, we can still define and analyse the above vector field globally. Note that this quantity equals 0 if and only if a point configuration $\omega \subset \Lambda$ (up to translation and rotation) is used to produce such a V^ω as in (1.2). As we will now see, there are defective configurations that do not permit this problem formulation, but are still locally like Λ.

1.2.2 Defining Order: Rotational Symmetry

We now consider a configuration described by Figure 1.2, describing a rotational defect, known as a disclination (Romanov and Vladimirov [1983]). As before there is no global bijection from this configuration to a punctured subset of the lattice $\mathbb{Z}^2$. In fact, we can see that even the edge labelling scheme assumed in the case of the translational defect is ill-defined. This means that for any covering $\{S_i\}_{i=1}^J$ and local displacement maps u_i^ω, we end up with the relation

$$u_{i+1}^\omega - \gamma_i u_i^\omega = \lambda_i \in \Lambda \tag{1.4}$$

where necessarily $\gamma_i \neq I$ for some $i \in 1, ..., J$. This means that there is no global V^ω defined through $V^\omega = \nabla u_i$ that is curl-free on the "locally lattice-like" region, which will be proved later. We find

$$\operatorname{supp} \operatorname{curl} V^\omega = \ell,\ \operatorname{curl} V^\omega \in H^{-1}(\cup T^\omega, \mathbb{R}^{2\times 2}),$$

where ℓ is some contour made up of connected edges of tiles, and starts at some vertex lying on the boundary of a "defect". This occurs for any choice of covering and any attempt at upgrading a local labelling scheme to a global one: on some overlap of two regions, the difference of gradients ∇u_i^ω will not be rank-one connected and this will be irreparable. We must choose the same edge to map to in each of the simply connected regions S_i to define our map that is locally a gradient, and can be seen from inspection this is not possible. Even though the edges above have an inconsistent labelling, locally we can always choose some γ_i so that V^ω can be defined on $S_1 \cup S_2$ as long as this region is simply connected. In some sense the local labelling of edges we choose is not physically relevant. This fact was missing from the translational case, where we arbitrarily chose some global reference frame with which to decide how to label edges. This degeneracy should be explicitly incorporated into any problem formulation in order to handle rotational defects.

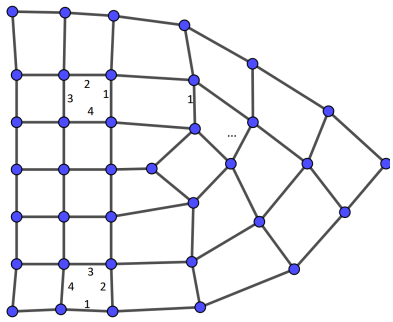


Figure 1.2: A rotational defect, known as a disclination. If we try to label the edges of a tile then propagate this to the others, the resultant labelling is inconsistent unlike the case for dislocations (c.f. Figure 1.1).

We introduce the vector fields

$$L^2(U,\Gamma) = \{\gamma \in L^2(U) : \gamma(x) \in \Gamma \text{ for all } x \in U\}$$

We will work with these vector fields rather than the constant rotation matrix γ_T as found in (1.3). We will consider the following problem:

Order In The Presence of Rotational Defects

Let $\{S_i\}$ be a covering of disjoint sets and let $\{V_i^\omega\}$ be the gradients of the local displacement maps. Define the vector field $V^\omega : \cup T^\omega \to \mathbb{R}^{2\times 2}$ as above with $\operatorname{curl} V \in H^{-1}(\cup T^\omega)$. Note for any simply connected S there exists $\gamma_S \in L^2(S,\Gamma)$ with $\operatorname{curl}(\gamma_S V) = 0$ on S. We define the problem of estimating such a field's orientational order by the following. For vector fields $V^\omega \in L^2(\cup T^\omega, \mathbb{R}^{2\times 2})$, we consider

$$\text{for } V^\omega: \text{ for all simply connected } S,\ \exists \gamma_S \in L^2(S,\Gamma) : \operatorname{curl}(\gamma_S V) = 0 \text{ on } S$$

$$\text{estimate} \min_{R\in \mathrm{SO}(2)} \min_{\gamma \in L^2(T,\Gamma)} \|V^\omega - \gamma R\|_{L^2(\cup T^\omega)}. \tag{1.5}$$

Just as before, for V_i^ω produced from local bijections from the configuration to regions of the lattice, the quantity in (1.5) above equals 0 if and only if $V^\omega \in \Gamma$ everywhere. Note however that since we do not require V^ω itself to be a gradient locally, this does not mean V^ω is constant. This removes the degeneracy in needing to pick a reference rotation for the whole configuration and allows an analytical treatment of rotational defects. For instance, for a perfect subset of the square lattice, arbitrarily giving each tile its own edge labelling compared to propagating the same one to the other tiles results in an equivalent quantification of the configuration's order. This is demonstrated in Figure 1.3.

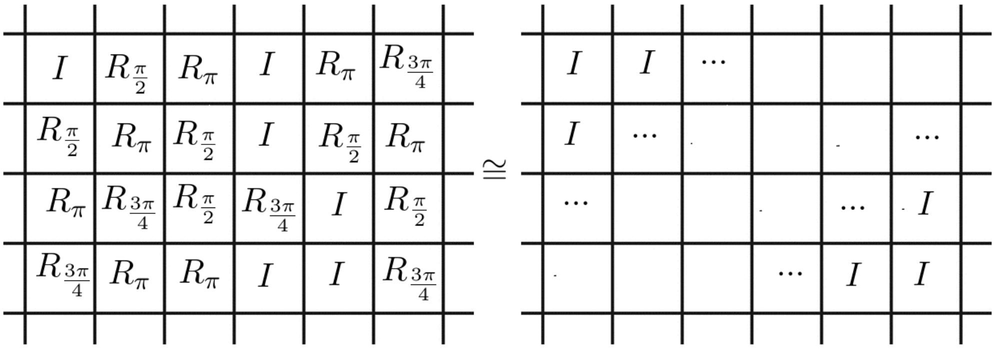


Figure 1.3: It should not matter whether any algorithm for deciding V^ω produces values rotated by differing elements of the symmetry group Γ.

While it requires more notation than the case for translational defects, we will see that in this framework we can again recover the presence of a rotational defect by the irremovable jump condition in (3.3). This definition incorporates translational defects.

1.3 Orientational Ordering in Statistical Mechanics

We now define what we mean by orientational ordering in a statistical sense based on the conditions above. We briefly review a paper that has explored this notion, and then introduce generalisations to both analytical estimates and statistical results for this problem. Throughout this thesis we will work with the square lattice $\mathbb{Z}^2$. Let $U_n = n[0,1]^2$ equipped with periodic boundary conditions. We will consider point configurations $\omega \subset U_n$ that satisfy the following conditions, and collect these ω into the set $\tilde{\Omega}_n$:

1. For each ω there exists a unique connected region $\cup T^\omega$ made up of "locally lattice-like" tiles and $D^\omega = U_n \setminus \cup T^\omega$
2. On T^ω there exists an overlapping covering $\{S_i\}$ and collection of piecewise affine maps on each S_i so that $u_i : S_i \to M_i$ is a continuous bijection with $u_i(x) \in \mathbb{Z}^2$ for each $x \in S_i \cap \omega$, and $M_i \subset \mathbb{R}^2$.
3. There exists a vector field $V^\omega \in L^2(\cup T^\omega)$ with $\operatorname{curl} V^\omega \in H^{-1}(\cup T^\omega)$ so that $\gamma_i^\omega V^\omega$ is the gradient of one of the above maps, for some $\gamma_i^\omega \in L^2(S_i, \Gamma)$.

We say $\omega \in \tilde{\Omega}_n$ if ω satisfies the three above conditions. Suppose now we are given an energy $H(\omega)$ defined on $\cup_n \tilde{\Omega}_n$ that is translation and rotationally invariant, $H(\Lambda_n) = 0$ and

$$H(\omega) = \sum_{t \in T^\omega} H_l(t) + \sigma|\partial D^\omega|, \quad H_l(t) \geq c_1 \|\mathrm{dist}(\nabla u_i, \mathrm{SO}(2))\|^2_{L^2(t)}. \tag{1.6}$$

Here $\sigma > 0$ is a parameter that penalises the number of tile edges in the boundary of the defect set D^ω. Moreover, t is a tile of some appropriate locally lattice-like tiling T^ω and $\nabla u_i, i \in \{1, ..., 4\}$ is an arbitrary choice from the four gradients obtained from piecewise affine maps from t to $t_0 = [0,1]^2$. Suppose μ is some probability measure on $\tilde{\Omega}_n$. Define the partition function and expectations

$$Z_{\sigma,\beta,n} = \int_{\tilde{\Omega}_n} e^{-\beta H(\omega)} d\mu, \quad \mathbb{E}_{\sigma,\beta,n}(\cdot) = Z^{-1}_{\sigma,\beta,n} \int_{\tilde{\Omega}_n} (\cdot) e^{-\beta H(\omega)} d\mu. \tag{1.7}$$

Definition 1.3.1. *We say that $\tilde{\Omega}_n$ exhibits orientational ordering if for all $\sigma > \sigma_0$,*

$$\lim_{\beta \to \infty} \limsup_{n \to \infty} \mathbb{E}_{\sigma,\beta,n} \left[\min_{R \in \mathrm{SO}(2)} \min_{\gamma \in L^2(T^\omega, \Gamma)} |T^\omega|^{-1} \|V^\omega - \gamma R\|^2_{L^2(T^\omega)} \right] = 0,$$

where expectation is defined as in (1.7)*. In a situation where all configurations have a consistent scheme to label edges, this reduces to the statement that for all $\sigma > \sigma_0$*

$$\lim_{\beta \to \infty} \limsup_{n \to \infty} \mathbb{E}_{\sigma,\beta,n} \left[\min_{R \in \mathrm{SO}(2)} |T^\omega|^{-1} \|V^\omega - \gamma_i R\|^2_{L^2(T^\omega)} \right] = 0, \tag{1.8}$$

where $\gamma_i \in \mathrm{SO}(2)$ is some fixed choice of rotation by $i\frac{\pi}{2}$ and $\operatorname{curl} V^\omega = 0$ in $\cup T^\omega$.

This is the only definition of orientational ordering we consider. While significant work could be done in exploring its relation to other kinds of order, this is the definition we study as it can be attacked analytically, and the analysis of the quantity on the left hand side for as large a class of vector fields as possible makes up the bulk of this thesis. The statistical task for us is to demonstrate orientational ordering in this specific sense for as large a subset of configurations $\Omega_n \subset \tilde{\Omega}_n$ as possible. We begin by reviewing current results on this task.

1.4 Orientational Ordering in the Literature

In Aumann [2015] a model of a crystal is considered where the energy is of the same form as Equation (1.6). In many ways it is more general than the models discussed above: it is defined in any dimension larger than two, and allows for more complicated ground states than a single lattice. However, there are some limitations and technical details to discuss.

- To begin with it is not clear if the construction of the tiling mentioned in Item 1 of Section 1.3 is not necessarily unique. It is a multi-step process, and in the case of a degenerate tiling one is chosen uniformly at random. The energy may then be ill-defined for certain configurations.

- It is claimed without proof that Item 2 allows the construction of a single-valued field V^ω with $\operatorname{curl} V^\omega = 0$ on $\cup T^\omega$. The non-uniqueness of mappings due to rotational symmetry is not explicitly mentioned.

- The conditions in Aumann [2015] implicitly rule out rotational defects and vector fields with the described properties in Item 3. That is, a consistent edge labelling is implicitly assumed to exist on any connected region of a configuration.

For such configurations the following is demonstrated, using the concept of orientational ordering for translational defects (1.3) above:

Theorem 1.4.1. *(Orientational Ordering: Aumann) Assume the above notions can be made rigorous. Then there exists some $\sigma_0 \in \mathbb{R}_+$ such that for all $\sigma > \sigma_0(n) = O(n^2)$*

$$\lim_{\beta\to\infty} \limsup_{n\to\infty} \mathbb{E}_{\beta,n}\left[\frac{1}{|T^\omega|} \min_{\mathrm{SO}(2)} \sum_{t\in T^\omega} \|V^\omega - R^\omega\|^2_{L^2(t)}\right] = 0.$$

Remarks: While allowing for defect sets D^ω to be arbitrary in size and shape, the above result requires the defect penalisation σ to increase with box size. Asymptotically then, it is evident that defects will be punished so harshly so as to not be present in some finite density for large configurations at any fixed temperature. Clearly, the first step for future work on this model is to produce the same results for a fixed, finite σ_0. There are also more fundamental questions to do with the mathematical underpinnings of the model and how to generalise it to include a finite density of different topological defects as discussed above. We now discuss the main tool that is used to prove this and similar claims, a *rigidity estimate* that allows us to compare a system's order to its energy.

1.5 Rigidity and Ordering

The main analytical estimate considered and generalised in this thesis originated in Friesecke et al. [2002]. It can be stated as follows. For all $u \in H^1(U, \mathbb{R}^2)$ where U is a Lipschitz domain there exists some constant rotation $R \in \mathrm{SO}(2)$ such that

$$\|\nabla u - R\|_{L^2(U)} \leq C_{RIG}(U)\|\mathrm{dist}(\nabla u, \mathrm{SO}(2))\|_{L^2(U)}, \tag{1.9}$$

with the same constant for all domains $\eta U, \eta > 0$. The estimate provides a means to compare the L^2-distance of the gradient of a function from the constant set of rotations to its pointwise one. It is evident that this is a useful tool in attempting to study (1.3) or (1.5) given the form of Hamiltonian (1.6). This notion forms the basis for demonstrating results in Heydenreich et al. [2014], Aumann [2015] and herein. As previously discussed however, it is evident the objects in the inequality (4.1) are not well-defined for defective configurations. Even if this could be resolved, without an extension procedure from $\cup T^\omega$ to U_n, we would have an inequality

$$\|V^\omega - R^\omega\|_{L^2(\cup T^\omega)} \leq C^\omega_{RIG}(\cup T^\omega)\|\mathrm{dist}(V^\omega, \mathrm{SO}(2))\|_{L^2(\cup T^\omega)},$$

where we must now quantify a constant in an analytical estimate for each defect configuration. For this reason an extension procedure to receive a vector field $\tilde{V}^\omega : U_n \to \mathbb{R}^{2\times 2}$ is useful. It gives us a fixed rigidity constant (recalling its scale invariant behaviour). However it cannot be expected that $\mathrm{curl}\, V^\omega = 0$ in D^ω. An estimate for extended vector fields incurs some term involving $\mathrm{curl}\, \tilde{V}$. When $V, \mathrm{curl}\, V \in L^2(U)$ for some Lipschitz domain U, it is shown in Aumann [2015] for general p and Müller et al. [2014] for $p = 1$ that

$$\|V - R\|_{L^2(U)} \leq C\|\mathrm{dist}(V, \mathrm{SO}(2))\|_{L^2(U)} + C(U, p)\|\,\mathrm{curl}\, V\|_{L^p(U)} \tag{1.10}$$

where the constant in front of the curl term either is not uniform for large domains, leaving us unable to use the same constant for each n in our statistical model, or the measure $\lambda(D^\omega)^{1/p}$ scales in a disadvantageous way for producing results regarding ordering in large n-limits. In our analysis we will adapt the rigidity estimates in the literature, as well as variants of them for domains with small holes or cuts (Scardia and Zeppieri [2012]) to better reflect both the discrete symmetry of the underlying lattice $\mathbb{Z}^2$ as well as thermalised models of crystals with "small defects" in them. Once the appropriate generalisations to gradients and curl free vector fields have been introduced, it will be shown that rigidity estimates of the form (1.10) are not sharp for a certain class of vector fields with prescribed curls. Along with this we will give a rigidity estimate for vector fields that describe rotational defects. This will allow us to demonstrate results similar to Theorem 1.4.1 with fixed σ_0 as well as make some statements about configurations with rotational defects.

1.6 Results: σ-Uniform Ordering

1.6.1 Admissible Configurations

Following the work of Aumann [2015] we will also assume many of the same conditions on configurations. For a full definition of these configurations see Section 2.12. While we cannot demonstrate the main result for the full set of configurations $\tilde{\Omega}_n$, we can for an appropriate subset Ω_n. We say a set of points $\omega \in \Omega_n$ if

- D^ω can be broken down into disjoint sets that have a minimum and maximum size
- Each ω possesses a consistent ordering, that is we may choose γ to be constant in (1.8) and define a vector field V^ω describing the strain of ω
- $|V^\omega|_\infty < M_1$ uniformly on $\cup T^\omega$

We also assume some conditions on the defect set D^ω. Fix $\alpha > 0$. Specifically, we assume that D^ω has a disjoint partition into sets D_0^ω and D_p^ω representing clusters and pairs of defects. These defects are such that

$$D_0^\omega \subset \cup_i B_\alpha(x_i^\omega), \oint_{\partial B_\alpha(x_i)} V^\omega \cdot dl = 0 \text{ for all } i,$$

and that $D_p^\omega = \{(d_1, d_2), ..., (d_{2K(\omega)-1}, d_{2K})\}$ for some $K(\omega) \in \mathbb{N}$ such that

$$\int_{\partial d_k} V^\omega \cdot dl = -\int_{\partial d_{k+1}} V^\omega \cdot dl.$$

Moreover we assume the following mutual spacing condition:

$$\text{for each pair } (d_k, d_{k+1})$$
$$\exists \rho(\omega) : C\rho(\omega) \geq \text{dist}(d_k, d_{k+1}) > \rho(\omega) \text{ for all } k.$$

That is, the defect set consists of clusters of defects that "screen" each other at a fixed length scale. Here screening means that in a sufficiently large contour enclosing a defect cluster, the net Burgers vector around this cluster will sum to 0. As well as screened defects, the mutual spacing condition allows for a set of defects distributed in the box U_n that also pair up at another (random) length scale. We call the latter defects dipoles. It includes dipoles whose length scales with the box width n. However, there would be few dipoles in number for such a configuration, in addition to any number of screened defect clusters that match the above conditions.

1.6.2 Orientational Ordering

With this in place we demonstrate the following result:

Theorem 1.6.1 (Uniform Orientational Ordering)**.** *Assume as above that the model in Section 1.3 is equipped with the configuration space $\Omega_n : n \in \mathbb{N}$. Then there exists $\sigma_0 \in \mathbb{R}_+$ which depends only on model parameters (not n or β) such that for all $\sigma > \sigma_0$*

$$\lim_{\beta\to\infty} \limsup_{n\to\infty} \mathbb{E}_{\sigma,\beta,n}\left[\inf_{R\in SO(2)} \frac{1}{|T^\omega|}\|V^\omega - \gamma^\omega R\|^2_{L^2(T^\omega)}\right] = 0.$$

where V^ω is any local deformation field *of each configuration, and $\gamma \in L^2(\cup T^\omega, \Gamma)$ is some $\Gamma-$valued vector field for each ω (c.f.* (1.7) *for the definition of the expectation).*

Remarks: The previous result established in Aumann [2015], while allowing for defect sets D^ω to be arbitrary, required $\sigma_0 \sim O(n^2)+O(n)$. Our result is true for all σ larger than some fixed value σ_0 giving uniform estimates, and not differently penalising the same density of defects the larger the box becomes. Our model therefore allows for a finite density of non-trivial defects at positive temperature. While our result does restrict the class of defects and underlying periodic structure, we believe that our assumption of screened defects is physically relevant, and in this respect provides an interesting result. We also provide a more comprehensive mathematical underpinning for the model, including a unique tiling, a rigorous treatment of the regularity of V^ω, and a discussion of configurations where this regularity breaks down. Our model also fully accounts for the discrete rotational symmetry of the lattice $\mathbb{Z}^2$ as well its translational symmetry, making the path to further generalisations of this model more tractable. We also demonstrate the following result.

Theorem 1.6.2 (Energy Estimates for Configurations)**.** *For the model in Section 1.3 with configurations $\tilde{\Omega}_n, n \in \mathbb{N}$ (that is, configurations that may have rotational defects), for all $\sigma > 0$*

$$\lim_{\beta\to\infty} \limsup_{n\to\infty} \mathbb{E}_{\sigma,\beta,n}[H(\omega)] = 0. \tag{1.11}$$

Recall that configurations $\omega \in \tilde{\Omega}_n$ can have inconsistent labellings. For these configurations, we cannot control the quantity

$$\min_{R \in \mathrm{SO}(2)} \min_{\gamma \in L^2(\Gamma, \cup T^\omega)} \|V^\omega - \gamma R\|_{L^2(\cup T^\omega)}$$

in a statistical sense in terms of the expression in Theorem (1.11). Nevertheless, we can quantify these configurations' energies. That is, although we cannot deduce the ordering of a model in the full generality of Equation 1.3.1 we have established what should be a useful result in this direction. Examples of configurations in Ω_n and $\tilde{\Omega}_n \backslash \Omega_n$ can be found in Chapter 5. Obvious targets for future work are to remove the mutual separation condition and dipoles and to complete a statistical analysis of configurations that permit rotational defects. However as progress towards this we have restored their status as point defects in this framework (rather than working directly with an object whose curl is concentrated on a line) and begun the process of adequately describing their behaviour through rigidity estimates. We now provide an overview of some analytical results demonstrated in this thesis.

1.7 Analytical Results

Due to the additional notation needed, we do not state all of the analytical results of this thesis here. They can be found in Chapters 4 and 5. It is Lemma 1.7.2 that we use to demonstrate Theorem 1.6.1.

Theorem 1.7.1 (Geometric Rigidity for α-Screened Fields)**.** *Let U be a simply connected domain with a Lipschitz boundary. Suppose that $V, \operatorname{curl} V \in L^2(U)$ is such that the support of $\operatorname{curl} V$ can be covered by a disjoint union of balls $\cup B_r(x_i) \subset U$, $\min(\operatorname{dist}(B_i, B_j), \operatorname{dist}(B_i, \partial U)) > r_{\min}$ for all i and all $j \neq i$, and for all i*

$$\int_{\partial B_r(x_i)} V \cdot \mathrm{d}l = 0.$$

We say $V \in S_r(U; r_{min})$. For any $V \in S_r(U; r_{min})$, there exists a rotation $R \in \mathrm{SO}(2)$ such that

$$\|V - R\|_{L^2(U)} \leq C(U)(\|\operatorname{dist}(V, \mathrm{SO}(2)))\|_{L^2(U)} + \alpha C(r_{\min})\| \operatorname{curl} V\|_{L^2(U)}),$$

and $C(U) = C(\eta U)$ for all $\eta > 0$ and all $V \in S_r(\eta U; r_{\min})$.

Lemma 1.7.2 (Rigidity for Admissible Configurations)**.** *Take any ordered set of points $\{x_k\}$ satisfying $C\rho > \operatorname{dist}(x_k, x_{k+1}) > \rho$ for any $\rho > 2r$. Define paired sets*

$d_k = \{B(r, x_k), B(r, x_{k+1}\}$ *and the set* $D = \cup_k d_k$. *Define the set of vector fields*

$$A_p(U, r) = \{V : \exists \rho > 0,\ D : \int_{d_k} \operatorname{curl} V = 0 \textit{ for all } k\}.$$

Then for any vector field $V \in S_\alpha(U; r_m) \oplus A_r^p(U)$, $2r < \alpha$, satisfying $|\operatorname{curl} V|_\infty < M$ there exists a rotation $R \in \mathrm{SO}(2)$ such that

$$\|V - R\|_{L^2(U)} \leq C_1 \|\operatorname{dist}(V, \mathrm{SO}(2))\|_{L^2(U)} + \alpha C_2(M) \|\operatorname{curl} V\|_{L^2(U)},$$

where C_1, C_2 are the same for all $\eta U, \eta > 2r$.

1.8 Program: Demonstration of Orientational Ordering

In order to place the structure of the thesis into context we will explain the method used for demonstrating Theorem 1.6.1. While the main focus of the thesis is on analysis, we also offer some generalisations for the applicability of this method. We will follow the same basic strategy as found in Heydenreich et al. [2014] and Aumann [2015].

1. Demonstrate, via a global rigidity estimate (Heydenreich et al. [2014] and Aumann [2015]) or otherwise (herein) that

   $$e_\sigma(\beta) = -\limsup_{n \to \infty} n^{-2} \log Z_{\sigma, \beta, n}$$

   exists for some range of parameters $\sigma \in [\sigma_0, \infty)$, and is such that

   $$\lim_{\beta \to \infty} e_\sigma = 0.$$

2. Let V^ω some vector field constructed above for each ω. Difficulties in ensuring it has the correct regularity aside, the first step is to establish that there exists an extension of V from $\cup T^\omega$ to all of U_n.

3. Establish that

   $$H(\omega) \geq \|\operatorname{dist}(V^\omega, \mathrm{SO}(2))\|^2_{L^2(\cup T^\omega)} + \sigma |D^\omega|.$$

4. Produce a rigidity estimate of the form

   $$\min_{R \in \mathrm{SO}(2)} \|V^\omega - \gamma^\omega R\|^2_{L^2(\cup T^\omega)} \leq C(U_1) \|\operatorname{dist}(V^\omega, \mathrm{SO}(2))\|^2_{L^2(\cup T^\omega)} + E(\operatorname{curl} \tilde{V}^\omega)$$

where E is some functional of the curl of the extension of V. Without this, a rigidity estimate of the form

$$\|V^\omega - R\|^2_{L^2(\cup T^\omega)} \leq C(\cup T^\omega)\|\mathrm{dist}(V^\omega, \mathrm{SO}(2))\|^2_{L^2(\cup T^\omega)}$$

contains a random, unquantified constant (this is elaborated upon later).

5. Apply a rigidity estimate to the extension of V^ω, leaving us with the task of considering

$$H(\omega) \geq C(U_1)^{-1} \min_{R\in\mathrm{SO}(2)} \|V^\omega - \gamma^\omega R\|^2_{L^2(\cup T^\omega)} + C(E(\mathrm{curl}\,\tilde{V}^\omega) - \sigma|D^\omega|).$$

6. Demonstrate or choose σ so that

$$E(\mathrm{curl}\,\tilde{V}^\omega) \sim \sigma|D^\omega|$$

to obtain that for some parameter region that

$$H(\omega) \geq C(U_1)^{-1} \min_{R\in\mathrm{SO}(2)} \|V^\omega - \gamma^\omega R\|_{L^2(\cup T^\omega)}.$$

7. Take expectations and apply 1 to deduce that for $\sigma \geq \sigma_0$ that

$$\lim_{\beta\to\infty} \limsup_{n\to\infty} \mathbb{E}_{\sigma,\beta,n}\left[\min_{R\in\mathrm{SO}(2)} \min_{\gamma\in L^2(\cup T^\omega,\Gamma)} \frac{1}{|\cup T^\omega|}\|V^\omega - \gamma R\|^2_{L^2(\cup T^\omega)}\right] = 0.$$

We will follow the same program for demonstrating orientational ordering, with the goal of showing it occurs for a sigma that is uniform in both n and β for as large a class of configurations as possible. While we believe that entropic estimates on the likelihood of defects could improve the above results, this thesis is concerned mainly with demonstrating the analytical portions needed for this program and improvements to the result found in Aumann [2015]. We will also provide an analytical foundation for future statistical work on this class of models.

1.9 Thesis Contents

For the last part of the introduction we now make some comments on the structure of the rest of the thesis. As briefly mentioned earlier, the construction of local interpolants $u(x)$ and the deformation fields V^ω rests on defining a continuum domain that contains points from the configuration. In Chapter 2 we provide an explicit construction of this discretised domain for the square lattice, following the same principles of Aumann [2015]. A discussion of how the discrete translational and rotational symmetries of the square lattice affect the tiling, the definition of V^{ω}, and this vector field's regularity follow in Chapter 3. This chapter also contains a technical discussion of defective configurations.

Once this is established, we move to Chapters 4 and 5: the main analytical portion of the thesis. We state and prove the rigidity estimates above with a more in-depth discussion of the notation, scaling arguments, and norm estimation. We prove lower bounds on the non-linear energy of configurations with translational defects and provide some intuition for the case of rotational ones also. We also prove the rigidity estimate needed in Chapter 6 to prove Theorem 1.6.2..

The last two chapters provide the statistical and supplementary calculations needed to prove the main results. Along with the proof of Theorem 1.6.2, Chapter 6 includes a heuristic discussion of the energy and entropy of rotational and translational defects. It also provides a rigorous proof of the properties of $E_{\sigma,\beta,n}[H(\omega)]$ when configurations may not have a tiling with a consistent labelling. This then provides a partial analysis of configurations that include *rotational defects* such as disclinations (c.f. Subsection 1.2.2.).

In Chapter 7 we provide the necessary L^2- regularity results needed in the analytical chapters. These calculations are included to produce a self-contained thesis. The bibliography follows.

Chapter 2

Tiling a Point Configuration

2.1 Points and Tilings

In this chapter we develop the notation and results needed to transition between a set of points or atoms in space and a continuum domain associated to them. For reference here are the relevant objects we will define or make use of.

2.1.1 Notation For This Section

- ϵ: A small, positive parameter. $\epsilon > 0$ encodes the maximum "strain" allowed in a tiling
- ω: A locally finite set. $\omega \subset \mathbb{R}^d$
- U: A compact set.
- Λ: A lattice. e.g. $\Lambda = \mathbb{Z}^2$
- t_0: A reference tile. The convex hull of a point $x \in \Lambda$ and its nearest neighbours.
- t: A tile. Any convex set whose vertices are ϵ-close to a translated, rotated version of t_0.
- T^ω: A tiling. A finite set consisting of tiles whose vertices co-incide with the points in ω. This collection of tiles is "locally lattice-like".
- $\cup T^\omega$: The continuum domain associated with a tiling. This is defined as the union over all tiles in a tiling.

- D^ω The defect set. Implicitly defined by a choice of U, the defect set is the complement $U \backslash T^\omega$. It is the region of space surrounding the points in ω that are not "locally lattice-like".

2.2 Lattices and the Reference Tiling

In order to define and analyse the orientational ordering of a finite set of points ω we will compare it, locally, to some translation and rotation of the square lattice $\Lambda = \mathbb{Z}^2$. To do this we will use continuum methods (that is, estimates on vector fields defined on a continuum domain rather than discrete mathematics). Therefore, we require a means to translate between an atomistic and a continuum description.

Definition 2.2.1 (Reference Tile and Tiling)**.** *Let $t_0 = [0,1]^2$, $e_1 = (1,0), e_2 = (0,1)$. We say this tile is the reference tile. We then define reference tiling of the lattice to be the countable set (and its finite restriction to a finite area) to be*

$$T^{\mathbb{Z}^2} = \{t : t = t_0 + ke_1 + je_2 \ (k,l) \in \mathbb{Z}^2\},$$

$$T_n^{\mathbb{Z}^2} = \{t : t = t_0 + ke_1 + je_2 \ (k,l) \in [0,n]^2\}.$$

.

That is $T_n^{\mathbb{Z}^2}$ is a finite set consisting of translated copies of the reference tile. Note the following (trivial) properties of the tiling:

- given a fixed reference tile, the tiling is unique
- the vertices of any tile, which we denote $v(t)$, are such that $v(t) \subset \mathbb{Z}^2$
- for any subset $S \subset T^\omega$ whose union is simply connected, $v(S) \subset \mathbb{Z}^2$ is a simply connected set in $\mathbb{Z}^2$ (in the sense of graphs). That is, edges of tiles which share a point are such that their vertices share a nearest neighbour in $\mathbb{Z}^2$- the tiling respects the connectivity of the lattice.

Our goal is to generalise this to locally finite sets ω. In order to do this we will define the perturbation of a reference tile and what it means for a tiling made of perturbed tiles to be locally lattice-like.

2.3 Points, Tiles and Reference Tiles

We begin with the definition of *perturbed tiles*. Let $c = |v(t_0)|$ denote the number of vertices of the reference tile.

Definition 2.3.1 (A Tile). *We say a closed, convex set t is a tile if $|v(t)| = |v(t_0)|$.*

Definition 2.3.2 (Perturbations of t_0). *We say a tile t is an ϵ-perturbation of t_0 if there exists some $a \in \mathbb{R}^d$ and $R \in \mathrm{SO}(2)$ such that*

$$\mathrm{dist}(a + Rv(t), v(t_0)) < \epsilon.$$

where the distance is computed up to some relabelling of the vertex set $v(t_0)$. We define the set $N_\epsilon(t_0)$ to be the set of all ϵ-perturbations of t_0. We refer to these as the set of perturbed tiles for brevity.

We now discuss how to relate tiles to sets of points. Let $\omega \subset \mathbb{R}^2$ be some locally finite set of points in the plane and let $N_\epsilon(t_0)$ be given.

Definition 2.3.3. *Let $\omega_1, \omega_2, ...\omega_c \subset \omega$ be a set of points in the plane. We say these points form a perturbation of $v(t_0)$ if there exists $t \in N_\epsilon(t)$ such that $v(t) = \omega_1, ..., \omega_c$.*

We will use deformed tiles to produce a tiling $T^\omega \subset \mathbb{R}^2$ of configurations of points in the plane. T^ω will be a finite collection of tiles where $v(t) \subset \omega$ for all $t \in T^\omega$. We will use these tilings to define admissible configurations as we consider in the model of the crystal introduced later, as well as more general configurations.

2.4 Points and Tilings

For analytical purposes we will require configurations to possess a tiling that has certain properties that are locally similar to $T^{\mathbb{Z}^2}$. The following are goals we will need to meet in the construction of the tiling for it to be in harmony with the results found in Aumann [2015].

Goals for the Tiling T^ω:

- The tiling T^ω is well defined, i.e. it is unique and the same configuration always yields the same tiling T^ω
- we can define a value to each tile t so that we receive a single-valued vector field on $\cup T^\omega$
- on any simply connected region $S \subset \cup T^\omega$, there exists a single valued, continuous map v from S to a simply connected region $S^{\mathbb{Z}^2} \subset \cup T^{\mathbb{Z}^2}$ such that $v(\omega \cap S) \subset \mathbb{Z}^2$ and connected edges are mapped to connected edges in a way that preserves orientation.

- in any simply connected region, it is possible to give one tile an edge labelling e_1, e_2, e_3, e_4, that can be propagated to the other tiles uniquely (given the labelling of the chosen tile).

Goals 1-3 are similar to the properties met by the construction of a tiling in Aumann [2015]. However, therein a stronger version of the fourth goal is implicit, that it holds on any connected subset. This goal is needed to construct a unique, single valued vector field V^ω that is locally a gradient on an arbitrary connected, locally lattice-like tiling. Without this goal met, the construction of a single-valued vector field V^ω with the needed properties is ill-defined. These considerations lead us to the following construction as well as an examination of the properties of vector fields V^ω.

2.4.1 Construction of an Unrestricted Tiling $\tilde{T}^\omega$

Let $\omega \subset \mathbb{R}^2$ be a locally finite set of points[1]. Let t_0 be a reference tile and $\epsilon > 0$ be given.

Definition 2.4.1. *We define the unrestricted tiling $\tilde{T}^\omega$ of ω by the set of tiles*

$$\tilde{T}^\omega = \{t \in N_\epsilon(t_0) : \exists \underline{\omega}^t = \{\omega_1^t, ..., \omega_c^t\} \subset \omega : v(t) = \underline{\omega}^t\}$$

That is, this is the set of all perturbed tiles whose vertices lie exclusively on points in ω. Amongst other irregularities these tiles may overlap. As discussed above, without refining this tiling there exist many configurations we consider "defective" that have tiles attached to them.

Definition 2.4.2 (Continuum domain associated to a tiling)**.** *For any finite set T consisting solely of tiles $t \in N_\epsilon(t_0)$, we define*

$$\bigcup_{t \in T} t = \cup T \subset \mathbb{R}^2$$

While the definition of the unrestricted tiling does not need t_0 to be a square, and the concepts below can in principle be adapted to other reference tiles (see Aumann [2015]), to provide an explicit construction and avoid excessive notation we will only work with a square reference tile. Moreover, we will assume $\epsilon < \frac{1}{3}$ in the definition of a perturbed tile. This ensures that all perturbed tiles have the same

[1] The methods we use are only applicable in two dimensions. Generalisations that result in non-uniform statistical estimates can be found in Aumann [2015].

number of edges as t_0, and that all tiles $t \in N_\epsilon(t_0)$ are convex, as well as stopping tiles being able to "pack" too closely. Before we construct the restricted tiling we require we introduce some notation concerning labelling edges.

2.5 Edge Types, Labelling and Consistency

In order to classify how tilings can in some way be defective compared to $T^{\mathbb{Z}^2}$ we now introduce the concept of edge types and local labelling. This will allow us to define both translational and rotational defects in tilings.

Definition 2.5.1 (Edge type)**.** *Let t_0 be the reference tile. Label a vertex x_1 arbitrarily, and label the others $x_2, ..., x_c$ in an anticlockwise fashion.*

We assign the vectors $e_i = x_{i+1} - x_i$ where we consider the index $i \bmod c$ to the edges of t_0. We say an edge e in the tiling $T^{\mathbb{Z}^2}$ has type or label i if $e = x_{i+1} - x_i$ for some $i \in 1...c$ and x_i vertices of t_0.

These vectors are important geometrically, as counting their number or considering whether a *global* labelling is even possible allows us to identify the presence of defects. We use the edge type to define a local labelling in tilings T^ω. Due to the discrete rotational symmetry of the lattice there is an underlying arbitrary choice in which edge we label '1'. We will use the convention for the square lattice that the edge connecting $(1, 0)$ to $(1, 1)$ will be labelled as e_1.

Definition 2.5.2 (Labelling $T^{\mathbb{Z}^2}$)**.** *Pick any tile $t_0 \in T^\Lambda$ and label its four edges as described above. If t shares a whole edge with another tile t', label this edge of t' by $i + 2 \bmod 4$, where i is the label given to the edge when considered an element of t. Doing this inductively leads to one of four possible labellings of $T^{\mathbb{Z}^2}$.*

Definition 2.5.3 (Local Consistent Labelling)**.** *Let S^ω be a collection of tiles with non-overlapping interiors, and be such that $\cup S^\omega \backslash \omega$ is simply connected. Pick a tile $t \in S^\omega$ and label its edges in an anti-clockwise fashion as above.*

For every tile that exactly shares a whole edge e_i with t, label their shared edges $i + 2 \bmod 4$. We say S^ω possesses a consistent labelling if this labelling can be carried out inductively to all $t \in S^\omega$ such that

- *Every edge e belonging to the tiling S^ω has exactly one label*
- *If an edge e has type i, the edge connected to it anti-clockwise has type $i + 1 \bmod 4$ if it exists*

- *The resultant tiling does not depend on which tile is chosen first, only on one of the four ways to label the first tile.*

Definition 2.5.4. *We say a tiling T^ω has a consistent labelling if an edge labelling exists for the whole tiling T^ω, not just for simply connected subsets. We will refer to this as a globally consistent labelling if the tiling is multiply connected.*

It will turn out that all simply connected *restricted* tilings posses a consistent labelling, but counter-examples can be given for unrestricted tilings. Before discussing restricted tilings and labellings we introduce some notation regarding contours consisting of edges in a tiling.

2.5.1 Contours and Loops

In this subsection, we establish the notation for the equivalent of contours and closed contours to define and describe *defects* in a tiling.

Definition 2.5.5 (Contour)**.** *A contour is an ordered collection of edges of tiles in T^ω such that each edge shares one point with the previous one and this point lies in ω.*

Definition 2.5.6 (Loop)**.** *A loop is a closed contour, that is the last vertex of the last edge is equal to the first vertex of the first edge in the contour .We will work with an oriented loop where the labelling is anti-clockwise when summing and integrating over edges.*

We now turn to the construction of a restricted tiling T^ω that locally resembles the reference tiling $T^{\mathbb{Z}^2}$. We will provide examples as to why each restriction we make is necessary for locally defined, continuous bijections from $\cup T^\omega$ to $\cup T^{\mathbb{Z}^2}$ to exist.

2.6 Constructing the Restricted Tiling

In order to produce tilings that are locally like $T^{\mathbb{Z}^2}$ we will have to restrict the possible tilings we consider. To this end we begin by defining the set of *edge neighbours* of t, denoted $n(t)$, as follows:

$$n(t) = \{t' \in \tilde{T}^\omega : t' \neq t,\ t' \cap \{t \backslash (v(t))\} \neq \varnothing\}$$

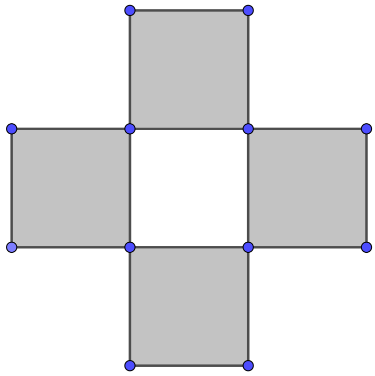


Figure 2.1: The set $n(t)$ for a reference tile. The shaded tiles are elements of $n(t)$, the white tile t is not.

That is, these are tiles that share an edge, part of an edge, or the interior of t (but ignores tiles that just share a tile corner). In the reference tiling $T^{\mathbb{Z}^2}$, we have

$$n([0,1]^2) = \{t_0 + (-1,0), t_0 + (0,-1), t_0 + (1,0), t_0 + (0,1)\}$$

See Figure 2.1 for a diagram. With this in place we define the sets

$$\begin{aligned} R_1(t) &= \{t' \in n(t) : t \cap t' \neq \text{ a whole edge}\}, \\ R_2(t) &= \{t : n(t) = \varnothing\}. \end{aligned}$$

$R_1(t)$ includes edge-neighbours of t whose interior overlaps with t, and tiles that only share part of an edge of t. $R_2(t)$ contains tiles that are completely isolated or only share a single vertex with another tile. We now consider a tiling

$$T_1^\omega = \tilde{T}^\omega \backslash \bigcup_{t \in \tilde{T}^\omega} \left(R_1(t) \cup R_2(t)\right).$$

This tiling has had isolated tiles, tiles whose interiors overlap, and tiles that occupy only part of an edge of a tile removed.

Lemma 2.6.1. *A tile t in T_1^ω has at most one edge neighbour per edge $e(t)$.*

Proof. Let t be a tile and let $t' \in n(t)$ be an arbitrary edge neighbour. Denote the edge where t intersects with t' by $e(t)$, and conversely the edge t' shares with t by $e(t')$. At least one such tile exists due to the definition of $R_1(t)$, and convexity of tiles guarantees they have only this edge in common. Since $\epsilon < 1/3$ the maximum length of the edge $e(t')$ of t' is strictly less than twice the minimum length of any other edge, including $e(t)$, i.e. $1+\epsilon < 2-2\epsilon$ iff $\epsilon < 1/3$.

This implies that if a tile t has an edge neighbour t', the edge $e(t')$ is shared in its entirety with t and no other tile. The intersection $e(t') \cap e(t)$ cannot be just part of $e(t)$ due to the definition of the set R_2. Moreover, t' cannot have an edge long enough to occupy a full edge of two separate tiles (and again, cannot occupy the whole edge $e(t)$ as well as part of an edge of another tile). $\square$

It turns out that the construction above is not restrictive enough to guarantee a "locally lattice-like tiling", as we will demonstrate diagrammatically. It is sufficient to note that in the reference tiling $T^{\mathbb{Z}^2}$, a tile that has a full set of edge neighbours is such that every vertex is shared by four edges in the tiling. T_1^ω allows for configurations where a tile can have a vertex shared by only three edges. Due to this fact we will now define the tiling we work with in later chapters by restricting T_1^ω further. As before we now consider the edge neighbours of an arbitrary tile $t \in T_1^\omega$:

$$n(t) = \{t' \in T_1^\omega : t' \neq t,\ t' \cap \{t \backslash (v(t))\} \neq \varnothing\}$$

Recall we denote the vertices of a tile t by $v(t)$. We define another restricting set

$$R_3(t) = \{t' \in n(t) : n(t') \cap n(t) \neq \varnothing\}.$$

That is, R_3 consists of tiles who share edge neighbours. Recall that $n(t)$ does not include t (to avoid trivial definitions). No tile of $T^{\mathbb{Z}^2}$ lands in R_3 since $t \notin n(t)$. Along with this we define the next-nearest neighbours of t:

$$n^2(t) = \{t'' : t'' \cap t \neq \varnothing, t'' \notin n(t), t'' \neq t\},$$

and the final restricted set

$$R_4(t) = \{t'' : t'' \in n^2(t),\ t'' \text{ is edge-connected to all } t' \in n(t) : t' \cap t'' \neq \varnothing.\}.$$

This set restricts configurations that contain "cracks" as explained below.

Definition 2.6.2. *We define the tiling T_2^ω of a point configuration ω to be*

$$T_2^\omega = T_1^\omega \backslash \bigcup_{t \in T_1^\omega} \left(R_3(t) \cup R_4(t)\right).$$

Lemma 2.6.3. *For any tile $t \in T_2^\omega$, the set*

$$B(t) = \{t' : t \cap t \neq \varnothing\}$$

has at most nine elements and forms a tiling with a consistent labelling. Moreover, every edge e_i that is not a boundary edge is edge-connected to another.

Proof. Let $t \in T_1^\omega$ be arbitrary. We begin by noting that $t \cup n(t)$ forms a consistently labelled tiling, and the union over all these tiles forms a simply connected set.

There are at most four and at least one tile in $n(t)$, and every tile in there shares exactly one whole edge with t by Lemma 2.6.1.

Arbitrarily label the edges of t by $1, 2, 3, 4$ anti-clockwise. For each tile $t' \in n(t)$ label the one edge it shares with t by $i + 2 \bmod 4$. No tiles $t', t'' \in n(t)$ are edge connected with each other due to the definition of R_3 (Equation 2.6). As they are only edge-connected to t there is no way for the labelling of $t \cup n(t)$ to be inconsistent.

We must now verify that we can propagate the labelling of $t \cup n(t)$ to the other elements of $B(t)$, as well as that there are at most four elements in $C(t) := B(t) \backslash (t \cup n(t))$.

If there are any tiles in $C(t)$ they must lie in $n(t')$ for some $t' \in n(t)$. There is at most one tile in $C(t)$ for each element t' of $n(t)$, whence there at most 4 elements of $C(t)$ in total. This follows from Lemma 2.6.1 applied to the tile t'.

We must now check that the tiles in $C(t)$ are appropriately edge-connected to the tiles in $n(t)$. Let any such tile be denoted t''. If t'' is edge connected with a tile t', it shares the entirety of the edge. Label this edge j. We propagate the labelling by the same rules above. If edge $j + 3 \bmod 4$ is shared between t'' and another element of $n(t)$ the labelling of $B(t)$ is complete.

The remaining possibility is that $t'' \cap t' \in v(t)$. This would be the case if the tile t'' shared a whole edge with $t'_1 \in n(t)$, but only a vertex with another tile $t'_2 \in n(t)$ (See Figure 2.4). However, this is impossible due to the restricting set R_4, as these tiles only share a vertex and not an edge.

Note that it is impossible for two tiles in $n(t)$ to be edge-connected with each other, because then they would have overlapping neighbour sets and fall foul of R_3. This would be the only way to generate an inconsistent labelling. $\square$

Definition 2.6.4 (Restricted Tiling)**.** *We define the restricted tiling T^ω to be the largest subset of T_2^ω that is a connected set (in the sense that $(\cup T_2^\omega) \backslash \omega$ is connected). Should no such unique set exist, we define $T^\omega = \varnothing$.*

It is then immediate that every ω with a non-empty tiling T^ω has a unique one. We will demonstrate these tilings are *locally lattice-like* in a specific sense, and point out that the global behaviour of these tiles is not sufficiently regular for our purposes without additional assumptions. We first discuss the construction of the tiling and why other assumptions lead to configurations that are not lattice-like.

2.7 Regular and Locally Lattice-Like Tilings

2.7.1 Regularity of a Tiling

As in Aumann [2015] we now introduce the definition of locally lattice like tilings using bijections. However, we separate some technical conditions used in the definition into a separate one.

Definition 2.7.1. *We say a tiling T^ω is ρ-regular if distinct edges and disjoint tiles belonging to T^ω have a fixed, minimum separation- in the sense that for any two distinct edges (e_1, e_2), there exists a point x on one edge e_1 such that* $\operatorname{dist}(x, e_2) > \rho$ *for some fixed ρ.*

2.7.2 Locally Lattice-Like Tilings

Definition 2.7.2. *We say a tiling T^ω is locally lattice like if there exists a family of subsets $T_1, T_2, ..., T_J \subset T^\omega$ for some $J \in N$ and a family $M_1, ..., M_J \subset T^{\mathbb{Z}^2_n}$ such that there exist continuous bijections*

$$v_j : \cup T_j \to \cup M_j,$$

mapping each tile t to a tile $Rt_0 + a$ for some $a \in \mathbb{R}^2, R \in \mathrm{SO}(2)$. Moreover, we require that

$$T^\omega = \bigcup_{j=1}^{J} T_j$$

and that the sets overlap. If $T_j \cap T_j \neq \varnothing$, the intersection consists only of whole tiles $t \in T^\omega$ and for every T_j there is some T_k such that their intersection consists only of whole tiles.

We postpone the proof that the restricted tiling we have constructed is locally lattice-like until Section 2.9. We first show that weakening the criteria used to construct it leads to configurations that are intuitively not "lattice-like" in certain places. In order to provide a more elementary construction we have not used bijections nor demanded a minimum separation of disjoint tiles. These are results of the construction rather than demands on the configuration as we will see. This allows us to classify defects without making reference to bijections or vector fields. However, defining an appropriate subset of point configurations we term *admissible configurations* will require some regularity assumptions.

Lemma 2.7.3. *Assuming that* $\mathrm{int} t \cap \omega = \varnothing$ *does not lead to a unique, lattice-like tiling* T^ω *for arbitrary configurations*

Proof. See Figure 2.2. □

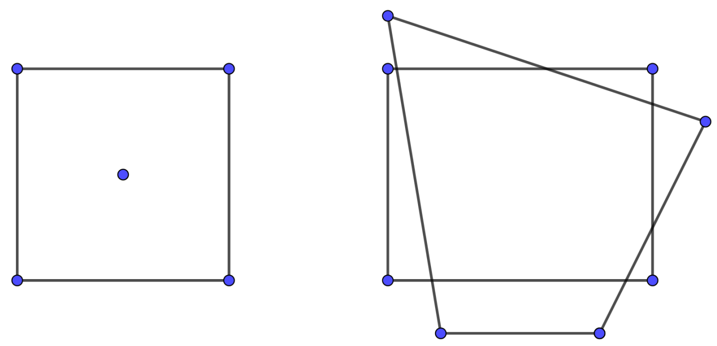


Figure 2.2: Assuming that the interior of a tile contains no point in ω does not assist us in defining a unique tiling.

Isolated points that do not generate tiles cause no problems, and assuming $\mathrm{int}\, t \cap \omega = \varnothing$ is unnecessarily restrictive. However, the tiling on the left is of course not like the lattice tiling. To exclude this configuration we would need to place a hard-core constraint on the relative positions of atoms. As we wish T^ω to be defined on all point configurations, this is not an option. The interior of two distinct tiles must then be disjoint.

Lemma 2.7.4 (Unrestricted tilings do not have locally consistent labellings)**.** *It is necessary to restrict tilings in order for simply connected tilings of point configurations to have a consistent labelling.*

Proof. See Figure 2.3.

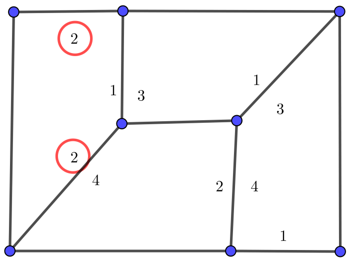


Figure 2.3: While for this tiling S^ω we have $(\cup S^\omega)\backslash\omega$ is simply connected, its edges cannot be labelled consistently.

$\square$

Lemma 2.7.5. *Without assuming that corners of tiles cannot lie on edges of another, there are tilings made of elements of $N_\epsilon(t_0)$ that do not yield continuous maps into a sub-tiling of $T^{\mathbb{Z}^2}$ for any $\epsilon > 0$. Without the condition that next-nearest neighbours who share a corner but not an entire edge, there are again configurations with no continuous map v into $T^{\mathbb{Z}^2}$.*

Proof. See Figure 2.4. Clearly there are no continuous maps v_1, v_2 that map the presented configurations to the sub-tilings of the reference tiling on the right-hand side. However, all configurations have a consistent labelling.

In the figure, every tile of the first tiling is a rigid body transformation of t_0. By scaling each configuration by a factor of $(1+\epsilon)$, each configuration is made up of elements of $N_\epsilon(t_0)$. It follows that any point configuration with similar connectivity that is tiled using elements of $N_\epsilon(t_0)$ would not possess a continuous map into an edge-connected sub-tiling of $T^{\mathbb{Z}^2}$ for any $\epsilon > 0$.

The second tiling, drawn with elements of $N_\epsilon(t_0)$, $\epsilon = 0.1$ shows that as defined a consistent labelling is not enough for a simply connected tiling to be locally lattice-like. The stricter condition that $B(t)$ as in Lemma 2.6.3 has a consistent labelling will be sufficient, however. $\square$

2.8 Interior Tiles and Defects

We now wish to use the scheme for labelling edges in the restricted tiling T^ω introduced in Section 2.5 to identify topological defects in configurations. This allows us to define an appropriate subset of all possible sets of points ω that we wish to consider.

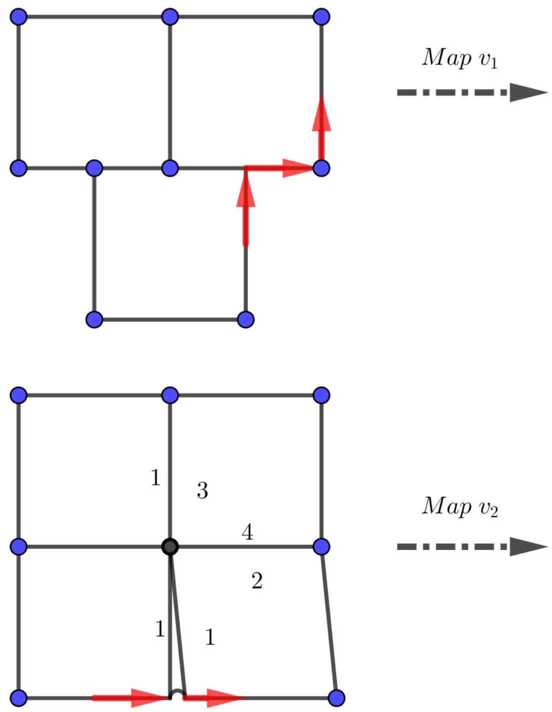


Figure 2.4: When edges are not shared in their entirety a failure for a continuous bijection to exist occurs. The contours and their image under a prospective bijection v_i are shown. In one space they are continuous, and discontinuous in the other.

From now on, T^ω without a tilde refers to a restricted tiling. An unrestricted tiling will be denoted using a tilde.

2.8.1 Bulk Tiles, Interior Tiles, and Boundary Tiles

Recall that we consider continuum domain associated to the tiling T^ω to be the connected set

$$\cup T^\omega := \bigcup_{t \in T^\omega} t.$$

Definition 2.8.1 (Bulk Tiles). *A tile $t \in T^\omega$ such that $\partial t \cap \partial \cup T^\omega = \varnothing$ is called a bulk tile.*

In addition to this we also define the set of boundary tiles that lie on the "edge" of a tiling.

Definition 2.8.2 (Boundary Tiles). *Let*

$$\partial T^\omega = \{t \in T^\omega : t \cap \partial \cup T^\omega \neq \varnothing\}$$

denote the set of boundary tiles.

Definition 2.8.3 (Interior and Exterior Boundary). *We say a tile t is an interior tile if it is a bulk tile, or there exists a loop $\ell \subset \cup T^\omega$ such that $t \subset \mathrm{hull}(\ell)$. If a tile is not an interior tile, we say it is an exterior boundary tile. We say interior tiles t such that $t \cap \partial T^\omega \neq \varnothing$ are interior boundary tiles.*

We will show that the bulk of a restricted tiling is regular and locally lattice-like. This will imply that tilings constructed on a torus rather than $\mathbb{R}^2$ and that only consist of "point" defects will be regular, locally lattice-like tilings, though we allow for more general defects in our model (under a regularity assumption to avoid technical difficulties).

Definition 2.8.4 (Defects). *We call the region enclosed by the interior boundary of T^ω the defects of T^ω, and denote it D^ω.*

2.9 All Restricted Tilings are Locally Lattice-Like

Lemma 2.9.1. *All restricted tilings T^ω are locally lattice like by construction.*

Proof. Recall that in Lemma 2.6.3 we demonstrated that for any tile $t \in T^\omega$, the set of t, its nearest and next-nearest neighbours denoted $B(t)$ is a set of at most 9 tiles, consistently labelled, and cannot contain a "crack". Let $j \in \{1, ..., J := |T^\omega|\}$ and label the tiles in the tiling arbitrarily using this index. The sets $B(t_j)$ will play the role of the subtilings T_j as in the definition of locally lattice like tilings.

We now establish that for each $T_j = B(t_j)$, that there exists a continuous bijection between $\cup T_j$ and $\cup M_j$, where M_j is an appropriately chosen subset of $B(t_0)$.

For each $t \in N_\epsilon(t_0)$ let ϕ_t^i, $i \in \{1, 2, 3, 4\}$ be piecewise affine bijections that map each edge of t to edge e_1 of t_0 respectively. Consider for some $t' \in n(t)$ the set $t \cup t'$. Let the edge they are connected by be labelled 1 on t, and therefore 3 on t' as $B(t)$ is consistent. Propagate this labelling to the other tiles in $B(t)$. We define the bijection $\phi : t \cup t' \to t_0 \cup (t_0 + e_1(t_0))$ by

$$\phi(x) = \begin{cases} \phi_t^1(x), \ x \in t \\ \phi_{t'}^1(x) + e_1(t_0), x \in t'. \end{cases}$$

By construction this is a piecewise affine, continuous bijection. Each of the bijections on the right maps into the reference tile in a way that preserves the edge labelling of $\{t, t'\}$ and the bijections have been shifted so that they form a continuous whole. For the other neighbours connected to $e_2(t), e_3(t), ...$ choose the bijection $\phi_t^1 + e_2(t_0), ...$ respectively. Repeat this process for elements of $n(t)$ to label the other remaining tiles should there be any, using consistency of the tiling to guarantee the maps take joined edges to joined edges.

It follows that there exists a continuous bijection from $\phi_j : \cup B(t_j) \to \cup M(t_0)$ where $M(t_0)$ has the same cardinality as $B(t_j)$. Clearly the collection $\{B(t_j)\}_{j=1}^J$ forms a covering of T^ω and consists of subtilings that form simply connected continuum domains. This yields a family of continuous bijections $\{\phi_j\}_{j=1}^J$ matching the needed criteria, the proof is finished. It follows that the restricted tiling T^ω is locally lattice-like. $\square$

2.10 Regularity of Tilings and Tile Defects

2.10.1 Interior Regularity

Lemma 2.10.1 (The Interior of a Restricted Tiling is Regular)**.** *For a fixed constant $\rho(\epsilon, t_0)$ that depends on ϵ, the lattice (in our case $\mathbb{Z}^2$) but not the point configuration ω considered, the interior of any non-empty restricted tiling is ρ-regular for all $\rho < \rho(\epsilon, t_0)$. The dependency of $\rho(\epsilon, t_0)$ on the lattice is based on the width of nearest neighbours. The constant for the lattice $r\mathbb{Z}^2$, $r \neq 1$ would not be the same.*

Proof. This follows from the lattice-like behaviour of the restricted tiling. For all tiles in the interior, $t \cap (\cup T^\omega)^c = \varnothing$. It follows that every tile in $\mathrm{int}T^\omega$ has a full set of neighbours. t and these tiles are not disjoint. Therefore for every tile t': $t' \cap t = \varnothing$, there is at least one tile in between. These neighbouring tiles cannot be arbitrarily small. The shortest path to a disjoint tile begins at a corner of t_0. The shortest path connecting t_0 to a point in t'' is a straight line, and one exists that passes through the edge of the tile t' (the restricted tiling as a whole is locally lattice like and this region is simply connected). The minimum length a side of a perturbed tile may have is $\ell_0 - \epsilon$ where ℓ_0 is the shortest length of a side of t_0. This allows us to choose $\rho(\epsilon)$ in the regularity constant. $\square$

2.10.2 Tile Defects

We now introduce the analogue of a *point defect* in this model. In models with defects they are often assumed to have no size. They represent the effects of small numbers of atoms that cause imperfections in a crystal (c.f. Ehrlacher et al. [2016]). True point defects such as interstitial atoms will have no tile attached to them in our model and cause no analytical concern. It can be shown that they do indeed contribute a small energy to the configurations. Since dislocations are usually modelled as having a strain $|V| \sim r^{-1}$ some regularisation must be used to ensure the objects of interest are square summable. The approach taken in many places such as Müller et al. [2014] is to introduce a cut-off proportional to an atomistic length scale.

This concept also appears in the formulation of the problem in this thesis. However, we are fortunate in that there is a length scale that enforces a minimum defect width if the defect is "small enough".

Definition 2.10.2 (Tile Defect)**.** *Suppose that a defect D^ω of T^ω is such that $D^\omega \subset t \in N_\epsilon(t_0)$ (where $t \notin T^\omega$). Then we say it is a tile defect.*

2.10.3 Boundary Regularity of a Tiling around Tile Defects

Lemma 2.10.3 (Tile Defects Lead to Regular Tilings)**.** *Suppose a restricted tiling T^ω is such that $D^\omega \subset t \in N_\epsilon(t_0)$ (where $t \notin T^\omega$). Then for all small enough $\epsilon > 0$ the tiling T^ω is ρ-regular. Here, $\rho(\epsilon)$ is the same for all ω that meet this condition and depends on ϵ.*

Proof. Let ℓ be the shortest loop surrounding the defect consisting only of edges of tiles from $N_\epsilon(t_0)$, and that it contains n edges. This in fact is the interior boundary of T^ω and consists of whole edges of boundary tiles. Call the tile that covers this defect t_D, i.e. $D^\omega \subset t_D$. Let $c = |v(t_0)|$. There are three cases we consider separately: $n = 3, n = 4 = c, n > 4$.

We begin by establishing the minimum and maximum angles between two edges of a tile $t \in N_\epsilon(t)$. We call the angle between two edges θ. Consult Figure 2.5. Here we have drawn two lines meeting at a vertex, then drawn the possible locations those two lines can end. By considering the case where $\epsilon = 0$ we can calculate the inner angle θ in the figure. Clearly the minimum and maximum angles are found by moving the edges when the edges are smallest, and moving the ends of the lines along the axis perpendicular to the bisector of the angle θ. finding the angle between the two edges is between $\frac{\pi}{2} - 2\phi$, $\frac{\pi}{2} + 2\phi$.

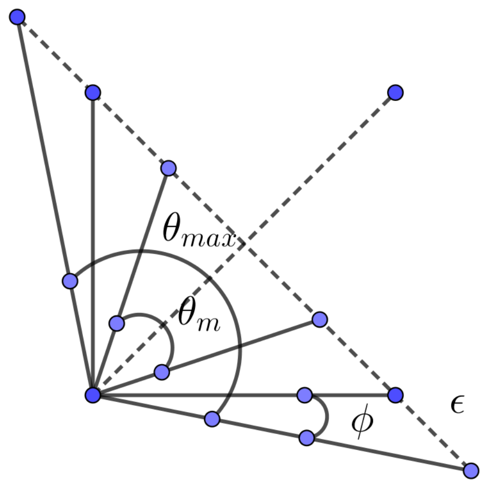


Figure 2.5: Finding the minimum and maximum angle between two edges.

After some simple algebra we find that

$$\phi = \arctan\left(\frac{\epsilon\sin(\frac{\pi}{4})}{1-\epsilon-\epsilon\cos(\frac{\pi}{4})}\right), \quad \theta \in \left[\frac{\pi}{2} - 2\phi, \frac{\pi}{2} + 2\phi\right].$$

A larger ϵ has a larger angular range. Numerically for $\epsilon = 0.25$ we find

$$\tan\phi = \frac{1}{3\sqrt{2}-1}, \quad \phi \approx 0.3084$$

and therefore $\theta \in (0.9549, 2.189)$, i.e θ lies between 54 and 126 degrees, where the lower and upper bounds are not sharp. We can use these bounds to rule out defects having arbitrarily small sizes due to the minimum length an edge may have. Note that this demonstrates all tiles $t \in N_\epsilon(t_0)$ are strictly convex.

Suppose $n = 3$. Then while none of the edges in ℓ are disjoint, always sharing one vertex, it is still true that the centre point of each edge has a minimum separation from the other two. There is no way to construct an arbitrarily small triangle using edges that must be edges of tiles in $N_\epsilon(t_0)$ for small enough ϵ. Every angle must be at least 54 degrees because each edge in the contour has two vertices shared by tiles in the tiling. Making the angle any smaller would deform these neighbouring tiles past their maximum angle. This is true for all boundary edges.

This gives the triangle a minimum height when combined with the minimum length $(1-\epsilon)$ of every side. Its base likewise must have this minimum width too.

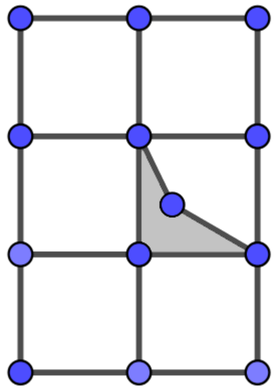


Figure 2.6: The shaded region causes the tile attached on the top right to fall foul of the restriction rules.

For $n = 4$ we have that the defect is strictly convex. If it were not, then it would not be allowed in the restricted tiling- such a shape constitutes a crack (see Figure 2.6). It then must be a strictly convex quadrilateral with sides that are sides of a tile, and therefore a tile itself. It then follows that disjoint edges have a minimum separation due to the fact that $\epsilon < \frac{1}{4}$ that all $t \in N_\epsilon(t_0)$ are strictly convex. It follows that a ball of sufficiently small radius ρ is compactly contained within t_D.

The regularity constant in this case can be chosen equal to this ρ, and is such that $\rho^{-1}(\epsilon) \to \infty$ as $\epsilon \to \frac{1}{2}$. It is only possible for edges of a tile to touch each other with $\epsilon = \frac{1}{2}$ or larger, and a priori there is no universal regularity for larger ϵ.

We now consider when $n \geq 5$, In this case ℓ forms an n-gon which must be contained inside a square equal to the boundary of t_D. To demonstrate this part numerically we will need a smaller ϵ than $\frac{1}{4}$. Arbitrarily choose a vertex x_1 and label its vertices anti-clockwise. x_1, x_2, x_3 form a "V" shape. For $\epsilon < \frac{1}{4}$ Turn this into a triangle by closing the remaining edge. Using the minimum angle above, this triangle has a minimum area (after some basic trigonometry)

$$A_T \geq \sin(\theta_m)\cos(\theta_m)(1-\epsilon)^2 > 0.47(1-\epsilon)^2.$$

Note that θ_m is larger for smaller ϵ, allowing us to use the same pre-factor for all $\epsilon < \frac{1}{4}$. Continue to find a total of $n - 2$ triangles. Some will be defined through 2 angles and a side. In this case the area is bounded below by an isosceles triangle with two minimum angles, and has a larger area than the above (as it as sine divided by cosine rather than multiplied, and the terms are both less than one).

There are $n-2$ such triangles. For this defect to be contained within a tile, its total area must be less than $(1+\epsilon)^2$, i.e.

$$(1+\epsilon)^2 > (n-2)0.47(1-\epsilon)^2, \ ; n \geq 5.$$

For $n=5$, we find that for this inequality to hold,

$$\epsilon > \frac{\sqrt{1.41}-1}{1+\sqrt{1.41}} \approx 0.086.$$

Choosing ϵ smaller than this rules out the existence of pentagonal or higher-sided tile defects. When combined with the other results, all remaining defects have a minimum size and so the tiling is regular up to the boundary.

Note that $\epsilon < 0.086$ is not sharp, and could be improved by calculating the minimum angle of smaller ϵ rather than using the one for the case $\epsilon = \frac{1}{4}$. The proof instead demonstrated there is a fixed, finite ϵ_0 guaranteeing regularity for $\epsilon < \epsilon_0$, with a numerical example. $\square$

Lemma 2.10.4. *Suppose that the defect set of a restricted tiling T^ω is comprised of disjoint tile defects $\{D_i^\omega\}_{i\geq 1}$ where each $D_i \subset t_i \in N_\epsilon(t)$, and for every D_i, D_j it is true that $(D_i \cup D_j)^c \subset \cup T^\omega$, that is the defects are at least separated by a whole tile or more. Then for small enough $\epsilon > 0$ the tiling is ρ-regular for some fixed $\rho(\epsilon)$ not depending on such ω.*

Proof. We apply the previous lemma and use separation of the defects assumed above. $\square$

The above demonstrates regularity in both the interior of a tiling, as well as regularity up to its interior boundary in the case of configurations with tile defects. There is in general no hope that ρ can be uniform outside of these circumstances. Figure 2.7 demonstrates an instance of the interior boundary and exterior boundary of a tiling being irregular. The interior boundary has a 'small' size in the first example. The reason $\rho-$regularity is required is to produce L^p and L^∞ estimates on a vector field $V : \cup T^\omega \to \mathbb{R}^{2\times 2}$. With some more work configurations with no exterior boundary can be absorbed into the statistical model considered later, by deleting boundary tiles and compensating for this difference with an appropriate error term. Configurations with irregular exterior boundaries are more difficult to analyse. We use periodic boundary conditions to eliminate such difficulties.

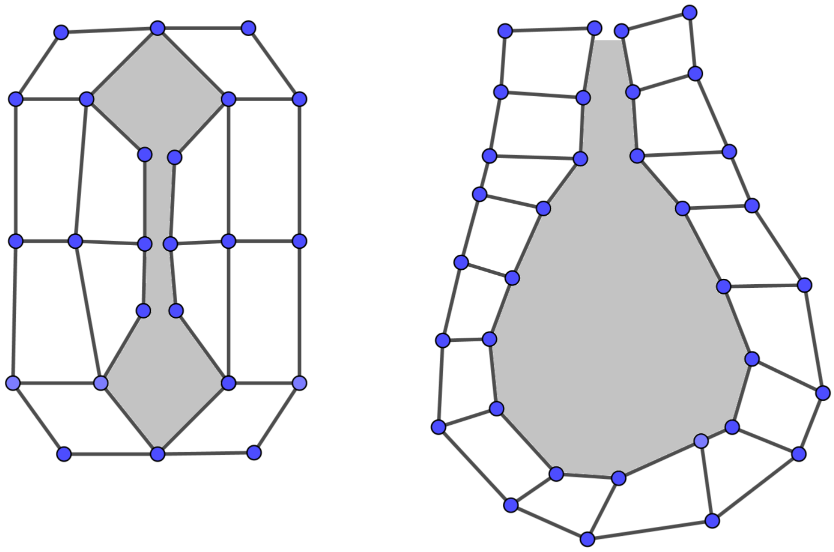


Figure 2.7: Configurations that are not regular up to the interior and exterior boundary respectively. For whatever $\epsilon > 0$ is chosen adding more tiles lets us create arbitrarily small bottlenecks. The gap between disjoint edges bordering the shaded region will be strictly smaller than those of any tile defect. This means there is no ω-independent, absolute regularity constant for any ϵ if we consider the space of all ω with restricted tilings (of large enough minimum cardinality).

2.11 Tile Defects and Discrete Symmetries

We begin this section with a note on tile defects with a more trivial effect on configurations:

2.11.1 Cavities and Tile Defects

Definition 2.11.1 (Cavities)**.** *Suppose a tiling T^ω possesses a defect region D^ω composed of tile-disjoint sets D_i^ω. Suppose further that each D_i^ω possesses a finite partition P consisting of elements of $N_\epsilon(t_0)$, and that T^ω has a consistent labelling along with*

$$\sum_{e_k \in \ell_i} e_k = 0$$

for any loop enclosing D_i^ω. We say these defects form cavities in the crystal. We let

$$\Omega_0 = \{\omega \subset \mathbb{R}^2 : \#\omega < \infty,\ \ D^\omega = \varnothing \textit{ or consists of cavities}\}.$$

These defects are not associated with the symmetry group of $\mathbb{Z}^2$ and still permit a global bijection from T^ω into the appropriate subset of $T^{\mathbb{Z}^2}$. As before, these form regular, lattice-like tilings. We now consider configurations such that $\tilde{T}^\omega$, the unrestricted tiling, covers all of $\mathbb{R}^2$ but $T^\omega \neq \tilde{T}^\omega$. This means that there are tiles that violate the conditions enforced by the restriction functions from Section 2.4. We will consider configurations such that the cardinality of all restricted tiles equals 1, that is $\bigcup_{t \in \tilde{T^\omega}} (R_1(t) \cup R_2(t)) \cup \bigcup_{t \in T_1^\omega} (\cup R_3(t) \cup R_4(t)) = 1$.

Definition 2.11.2 (Tile Defects)**.** *Suppose that T^ω is such that $D^\omega \in N_\epsilon(t)$. Then we say T^ω consists of a single tile defect. We denote the corresponding set of configurations ω by*

$$\Omega_1 = \{\omega \subset \mathbb{R}^2 : \#\omega < \infty,\ \ D^\omega \textit{ consists of a single tile}\}.$$

Lemma 2.11.3. *Configurations do not contain a cavity consisting of a single tile as a defect.*

Proof. We note $D^\omega \in N_\epsilon(t_0)$ and therefore its boundary is exactly ∂t for some $t \in N_\epsilon(t_0)$. Its vertices are points in the tiling and by assumption its neighbours are such that there is a continuous bijection from $\cup n(t)$ to a subset of $\cup T^{\mathbb{Z}^2}$. By mapping t to the tile that the tiles $\phi(n(t))$ surround we find that $T^\omega \cup D^\omega$ is a larger connected tiling that meets the conditions imposed by f, g, h. It follows that this tiling is larger than T^ω. $\square$

All of the configurations in Ω_0, Ω_1 are such that $\cup T^\omega$ is not simply connected. By construction, Ω_0 is the set obtained by assuming that $J = 1$ in the definition of locally lattice-like tilings. This allows a continuous bijection to be defined on contours that completely surround a defect, and for this reason we make no distinction between those configurations and configurations in which $D^\omega = \varnothing$. As we will see, Ω_1 consists of configurations that do not permit such a global bijection from T^ω to some region $M \subset T^{\mathbb{Z}^2}$ to exist. This is why in the definition of locally lattice-like tilings, a family of simply connected regions with a family of bijections was used. The failure of such a global bijection to exist is the result of the discrete symmetry group of $\mathbb{Z}^2$. We will now introduce the types of defects associated with restricted tiles in preparation for the next chapter.

2.11.2 A Translational Defect

As in the introduction, we now consider a defect of the form in Figure 1.3, referred to as a dislocation in the literature. A dislocation is contained within a loop ℓ if, after labelling edges (consistently), it is found ℓ contains an excess of one kind of edge. This excess when the loop is contracted as much as possible is the Burgers vector of a dislocation. We establish some facts about configurations with dislocations in them in order to motivate the discussion of the vector fields associated with them in later chapters.

Lemma 2.11.4. *A configuration possessing a dislocation has four consistent labellings, each associated to an element of the rotational symmetry group.*

Proof. By inspection, and the comments made in the introduction regarding the form of discontinuity between local bijections for translational defects. □

For each of the four possible labellings, we note that around every closed loop that encompasses D^ω, we have

$$\sum_{e_i \in \ell} e_i \in \mathbb{Z}^2$$

in fact, the sum is one of the four vectors that make up t_0 where the vector depends on the labelling chosen.

2.11.3 Two Translational Defects: Screening

The discrete rotational symmetry of the lattice means that for each configuration, the value that Burgers vectors take is decided by a specific choice of a rotation from

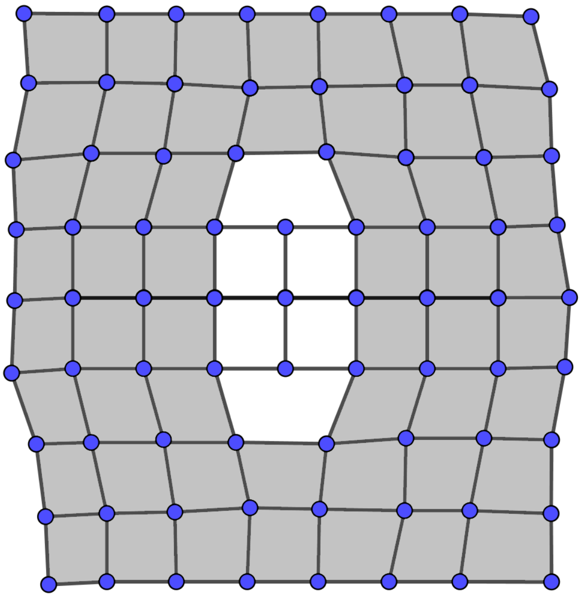


Figure 2.8: Two translational defects screen each other. There are the same number of edges on the top of the configuration as the bottom, and the same for either side.

Γ. However, regardless of this choice for each configuration, due to the fact that the labelling when (well-separated) translational defects exist is always consistent, the property that defects can *screen* each other always holds. This phenomenon is shown in Figure 2.8.

Lemma 2.11.5. *Suppose a region T^ω contains a single defect D^ω so that the edge sum around a loop enclosing D^ω equals* 0*, and that it is possible to consistently label every edge in T^ω. Then the interior (c.f. Definition 2.6.8) of the tiling T^ω is lattice-like.*

Proof. This can be done directly using the definition of locally lattice-like with $J = 1$ and counting tile edges, or to appeal to Helmholtz decomposition in a Sobolev space (Farwig et al. [2007]). □

The fact that configurations can screen each other in a way that there is no long-range topological defect to detect is extremely important to improving analytical and statistical estimates, as we will see in the next two chapters. This idea and the consequences of it appears in many areas of physics and mathematics, for instance in Müller et al. [2014], Kosterlitz and Thouless [1973], and Kosevich [2006]. We now discuss rotational defects to find a way to characterise them without appealing to bijections, as we have discussed for edge sums and dislocations.

2.11.4 Rotational Defects

We now discuss a defect that poses an analytical problem. Figure 1.5 in the introduction contains a simple configuration with a rotational defect, known as a *disclination* in the literature. Regardless of which convention for labelling the first edge $(1, 2, 3$, or $4)$ and regardless of which tile we begin with, we find that we cannot upgrade the local labelling to a global labelling. Travelling around a 1-tile thick contour surrounding the defect, we find that the tile labelling becomes rotated by γ. These configurations have no consistent labelling, and we can identify the presence of the rotational defect through this behaviour.

Definition 2.11.6. *We call the rotation matrix γ, the element γ that we must apply to an labelling on one side of the circuit in an inconsistent labelling to find the labelling on the other side (in an anti-clockwise sense) the Frank vector.*

This exposes the fact that a consistent labelling in a multiply connected tiling T^ω is genuinely a *global* property of the configuration, not a local one. It is why it was not used in the definition of locally lattice-like configurations. We will investigate the properties of bijections and vector fields for these defects later.

2.12 Admissible Configurations

We now use the above machinery to produce a class of configurations Ω_n for which an advantageous form of rigidity estimate can be demonstrated. These configurations will form the foundation of the statistical mechanical model introduced later on. Their definition makes use of the notation above. Their characterisation in terms of the vector field V^ω will also be given. We will continue to assume $\Lambda = \mathbb{Z}^2$.

Definition 2.12.1 (Admissible Configurations)**.** *Let $U_1 = t_0$ and let $n \in \mathbb{N}$. We define $U_n = nt_0 = [0, n]^2$. Equip this box with periodic boundary conditions. Let $\omega \subset U_n$ be a finite configuration in the box. Let T^ω be the restricted tiling of ω according to the construction in Section 2.4. Let $n_1 < n_2 \in \mathbb{N}$. Let $x \in U_n$. Let $\rho > 0$ be a given constant. We say ω is an admissible configuration if*

- *The restricted tiling is regular (c.f. Section 2.5), with a uniform regularity constant ρ for all ω*
- *Each ω possesses a consistent labelling, which we choose arbitrarily for each configuration.*

- *D^ω can be broken down into separated, disjoint sets that have a minimum size and maximum size. Denote each such set by d. Let $I \subset \mathbb{R}^2$ be a finite set of points such that $x \in D^\omega$ for all $x \in I$, and there is at most one point x belonging to each defect in the defect set. We assume there exists a partition of I into the sets I_0, I_p and numbers $r_m, \alpha_0, \alpha_p, \alpha_m$ such that*

$$D^\omega \subset \bigcup_{x \in I_0} B_{\alpha_0}(x) \cup \bigcup_{x \in I_p} B_{\alpha_p}(x)$$

That is there is a covering of the defect set by balls of two sizes, indexed by the sets I_0 and I_p respectively. This allows for a "cluster" of defects all inhabiting a ball of radius α_0, as well as smaller individual defects covered by balls α_p. As above we assume that

$$\textit{there exists } x \in d : B_{\alpha_m}(x) \subset d \;\; \textit{for all } d \in D^\omega.$$

i.e. all individual defects $d \in D^\omega$ have a minimum size.

- *We further suppose that for all $x \in I_0$ that*

$$\mathrm{dist}(x, y) > \alpha_0 + r_m \; \textit{for all } x, y \in I_0$$

$$\sum_{e^\omega \in \ell(x)} e^\omega = 0 \;\; \textit{for } x \in I_0$$

where ℓ is the smallest loop enclosing the union of the set $\{d : d \subset B_{\alpha_0}(x)\}$.

- *Let $D_p^\omega = D^\omega \cap B_{\alpha_p}(x)$, $x \in I_p$. We assume there exists a pair partition so that $D_p^\omega = \{(d_1, d_2), ..., (d_{2K(\omega)-1}, d_{2K(\omega)})\}$ for some $K(\omega) \in \mathbb{N}$ such that d_i is an individual defect for all i, and*

$$\exists s(\omega) : Cs(\omega) \geq \mathrm{dist}(d_k, d_j) > s(\omega) > 2(\alpha_p + r_m) \; \textit{for all } k, j \leq 2K(\omega)$$

$$\sum_{\partial d_k} e^\omega = -\sum_{\partial d_{k+1}} e^\omega, \;\; \left| \sum_{\partial d_k} e^\omega \right| \neq 0 \;\; \textit{for all } k$$

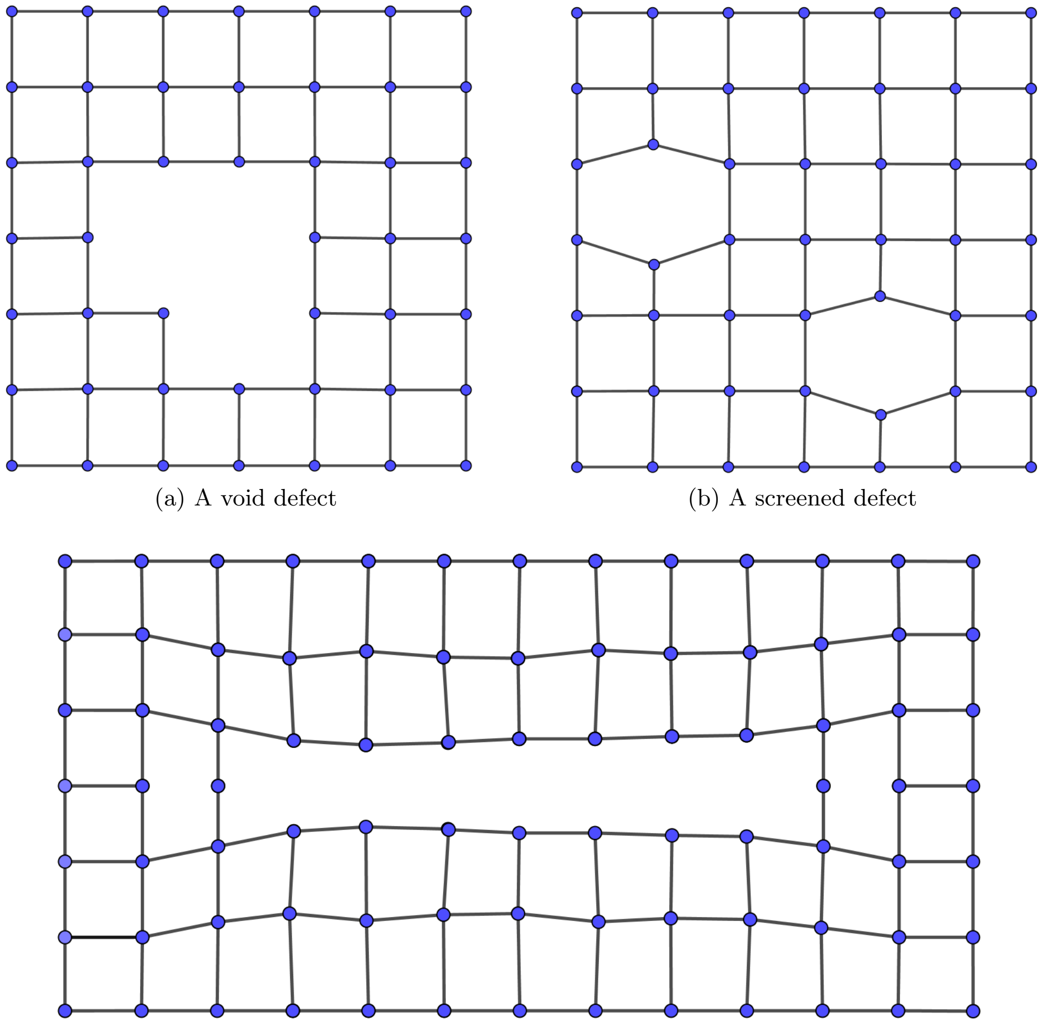
We call these paired defects. That is, for each ω the defects in D_p^ω all have some mutual separation s and each one is paired with another with an opposite Burgers vector. The separation $s(\omega)$ can be any large enough value and change for each ω.

We say each such ω is admissible, and collect every ω defined on U_n into the set Ω_n.

That is, the admissible configurations consist of well separated paired defects as well as clustered defects. The defect set consists of clusters of defects that "screen" each other at a fixed length scale, as well as a set of defects distributed in the box U_n that also pair up. We call the latter defects *dislocation dipoles*. The binding of dipoles is an important phenomenon in models with topological defects and points with similar interactions, in the previously referenced work by Kosterlitz and Thouless (reviewed in Kosterlitz and Thouless [1973]) as well as work in Brydges and Martin [1999] and Kosevich [2006]. These assumptions allow for dipoles that pair at any fixed length scale: for instance it includes dipoles whose length scales with the box width n, along with another fixed scale α. However, there would be few dipoles in number for such a configuration, in addition to any number of screened defect clusters that match the above conditions. Admissible configurations allow for the screened clusters to be much larger in radius than a single tile defect, but ultimately must have a uniform bound in size.

Lemma 2.12.2. *There exists large enough n and appropriate choice of fixed parameters above that there are ω whose defect sets are not empty. In fact, admissible configurations support a finite density of both screened clusters of defects as well as dislocation dipoles.*

Proof. Let $n \geq 6$. Consider the three building blocks below in Figure 2.9. Their perimeter exactly co-incides with a 6x6 or 12x6 'block" made of translates of the reference tile t_0. Along with a 6x6, 6x1, and 1x6 set of the reference tile t_0, we can assemble an admissible configuration with the building blocks for any $n \geq 6$. As long as for each element Figure 2.9 (c) there is an element above or below by Figure 2.9 (a) or (b) along with reference elements to fill the required length, then the dipoles will meet the mutual separation condition. Rotating any of these elements by a member of the rotational symmetry group $\Gamma(\mathbb{Z}^2)$ adds more admissible sub-tilings to assemble a larger one. Clearly we are free to choose any 6x6 defective block as at least half the elements in a row for large enough n, and place the dipole sub-tiling on every other row with at least two blocks between it and another on the same row. We can then see that Ω_n admits configurations with a finite density of screened and paired defects for appropriate parameter choices. $\square$



(a) A void defect

(b) A screened defect

(c) A defect pair

Figure 2.9: Building blocks to produce an admissible tiling.

Chapter 3

Local Bijections, Global Deformation and Discrete Symmetry

We will now introduce a means to describe defects using local bijections as in the definition of locally lattice-like configurations. While the defects themselves can be described only with the notation developed in the previous section (edge types and consistent orderings) we will ultimately consider the properties of these bijections from an analytical standpoint. They also make the role the discrete symmetry group of the lattice plays precise in terms of the curl of vector fields.

3.0.1 Local Bijections for Tilings

Definition 3.0.3. *Let t_0 be given and let $t \in N_\epsilon(t_0)$. Suppose $\phi : t \to t_0$ is a continuous bijection that maps edges to edges in an orientation-preserving way. For each of these bijections, there are three other associated ones where a given edge of t is mapped to each edge of t_0. This provides an enumeration of the rotational symmetry group $\Gamma(\mathbb{Z}^2)$. We enumerate the elements of Γ by $\gamma_1, \gamma_2, \ldots$. We define the functions $\phi_t^i(x) : \mathbb{R}^2 \to \mathbb{R}^2$ by*

$$\phi_t^i(x) = \begin{cases} \gamma_i \phi(x), x \in t \\ 0 \text{ otherwise.} \end{cases}$$

Since T^ω is locally lattice like, we have the following result:

Lemma 3.0.4. *Let S^ω be a simply connected tiling. There exist a collection of lattice vectors $\lambda_t \in \Lambda$ and a collection of rotations $R_t \in \Gamma(\Lambda)$ such that the function*

$$\phi(x) = \sum_{t \in S^\omega} \chi_t(x) \left(\lambda_t + \phi_t^{i(t)}(x) \right), \quad \chi_t(x) = \begin{cases} 1, x \in t, \\ 0, \ \textit{otherwise} \end{cases}$$

is a continuous bijection from $\cup S^\omega \to \cup M$, where M is a simply connected region in the reference tiling T^Λ. Since the λ_t are constants we include a characteristic function in the above. $i(t)$ is one of the four possible choices for a local displacement, and we may take different choices for each tile.

In the above, the λ_t and $\gamma_{i(t)}$ are symmetries of the lattice. Depending on the consistent ordering given to S^ω, the rotations will differ globally by one of the elements in the symmetry group. While this bijection always exists for simply connected regions, for multiply connected regions it may not. As we will see, ways in which the construction of the bijection fails to exist can be related to the properties of the λ_t and $i(t)$.

3.0.2 Local and Global Description of Local Deformation

We now wish to define a deformation field, a vector field $V^\omega \in L^2(\cup T^\omega, \mathbb{R}^{2\times 2})$ such that $\operatorname{curl} V^\omega = 0$ in the sense that $\operatorname{curl} V^\omega \in L^p(\cup T^\omega)$ and $\operatorname{curl} V^\omega = 0$ *a.e.*. Note that this is now a global object: a single valued vector field that in principle on the union of the whole tiling, in contrast to a family of separate global bijections. We will show that there exist locally lattice like configurations where this construction is not possible, which gave rise to the definition of the admissible configurations. To this end we define the local deformation of a tiling. To do this we have modified the definition of the local deformation in Aumann [2015]. As before, we start with a local construction of our candidate global description of a configuration's local deformation.

3.0.3 Local Bijections for Tilings

Definition 3.0.5. *Let S^ω be a simply connected tiling. Denote by $\lambda_t \in \Lambda$ a collection of lattice vectors and a collection of rotations $\gamma_t \in \Gamma(\Lambda)$ such that the function*

$$\phi(x) = \sum_{t \in S^\omega} \chi(t) \left(\lambda_t + \gamma_t \phi_t(x) \right)$$

is a continuous bijection from $\cup S^\omega \to \cup M$*, where* M *is a simply connected region in the reference tiling* T^Λ *with the same connectivity as* S^ω*. We define the tile gradient* $\nabla_t \phi$ *of a bijection to be the vector field*

$$\nabla_t \phi(x) = \begin{cases} \nabla \phi_t, x \in \mathrm{int}(t) \\ 0, \ \textit{otherwise.} \end{cases}$$

With this, we define the local deformation *of a simply connected tiling* S^ω *as the vector field* V_S^ω *in* $L^2(\cup S^\omega, \mathbb{R}^{2\times 2})$ *by*

$$V_S^\omega(x) = \sum_{t \in S^\omega} \nabla_t \phi(x) = \sum_{t \in S^\omega} \gamma_t \nabla_t \phi_t(x) \tag{3.1}$$

As before, for a fixed choice of tile bijections there are $|\Gamma|$ *choices of* ϕ *and* V_S*.*

It is important that S^ω is a simply connected tiling. If we instead performed this construction with a general restricted tiling T^ω, it can be that either ϕ fails to exist as a continuous function, or even the rightmost term in Equation (3.1) is poorly defined.

Lemma 3.0.6 (The Local Deformation is a Gradient)**.** *For a simply connected, restricted tiling* $\cup S^\omega$*, we have that* $\operatorname{curl} V_S^\omega \in L^2(\cup S^\omega, \mathbb{R}^2)$ *and* $\operatorname{curl} V_S^\omega = 0$ *a.e.*

Proof. Since ϕ is continuous and $V_S^\omega(x) = \nabla \phi(x)$ for the appropriate ϕ a.e., we find that $\operatorname{curl} V_S^\omega = 0$ on $\cup S^\omega$. ϕ exists as S^ω is locally lattice-like. □

The definition of the tile gradient will be of use when we discuss translational defects and extending the definition of V_S^ω to tilings with multiply connected continuum domains. When discussing a general restricted tiling T^ω and attempting to write Equation (3.1) down for this tiling, there are two main difficulties associated with the symmetries of the lattice.

Let $\{S_j^\omega\}_{j\geq 1}$ be a non-overlapping covering of a restricted tiling T^ω, so that each S_j^ω is simply connected. *Globally* define the local deformation of a tiling to be

$$V_T^\omega(x) = V_{S_j}^\omega(x), \ \ x \in \cup S_j^\omega$$

note that it is implicit in the definition that there is a choice of four possible local bijections for each simply connected sub-tiling S_j^ω as well as an infinite choice of shifts by lattice vectors. For certain tilings, V_T^ω is locally, but not globally, a gradient of some potential- regardless of what lattice shifts are chosen. We say the defects of T^ω that cause this behaviour are related to the translational symmetry group of $\mathbb{Z}^2$

for this reason. For other configurations, V_T^ω will possess a measure-valued in some region regardless of the choice of labelling for each sub-tiling. The exact nature of this curl is dependent on the rotational symmetry group of $\mathbb{Z}^2$, and so we will cause the defects that cause this behaviour rotational defects.

It is more convenient for various reasons, as in the definition of a locally lattice-like tiling, to work with an overlapping covering $\{S_j^\omega\}$ of a restricted tiling T^ω. While the preliminary definition of V_T^ω allows for an arbitrary choice of $\gamma_i \in \Gamma$ for each ϕ defined on $\cup S_j^\omega$, we are in fact not free to make more than on choice if we wish to define a single valued vector field $V^\omega \in L^2(\cup T^\omega, \mathbb{R}^2)$- since the S_j^ω overlap by definition, this fixes a choice of i for every other region S_j^ω if $V_{S_j \cup S_{j+1}}$ is to be single valued. If two regions S_j^ω, S_k^ω do not overlap but instead are adjacent to each other, different choices of γ for each bijection will mean the deformation will not be the gradient of a continuous vector field across the line connecting them. As before this will make it impossible to even globally define V^ω so that it is locally a gradient for certain configurations. We will see examples of these and analysis of them later.

3.1 Translational Defects And Local Bijections

We return to the dislocation found in Figure 1.3. We begin by noting the following result.

Lemma 3.1.1. *The configuration in Figure 1.3 has four consistent orderings, each associated to an element of the rotational symmetry group.*

Proof. By inspection. $\square$

For each of the four possible orderings, recall that around every closed loop that encompasses D^ω, we have

$$\sum_{e_i \in \ell} e_i \in \Lambda$$

in fact, the sum is one of the four vectors that make up t_0 where the vector depends on the labelling chosen. To fix notation, we will work with the same ordering as in the introduction. This means that summing the edge types reveals an excess of e_1. The translational defect can be described as a failure of a global continuous bijection from $\cup T^\omega$ to $\cup M^\Lambda$ (pictured below) to exist.

Let $\lambda_t \in \Lambda$ be a family of lattice vectors, one for each tile in T^ω. In the following, we let $\phi_t : t \to t_0$ be local bijections, where each local bijection maps the edges of tiles t to the edges of t_0 indicated by the labelling. Let $\ell = e_1, .., e_n$ be a loop enclosing D^ω. Denote $\ell_k, k \leq n$ to be the contour containing the first k edges of the loop ℓ. Let $S_k^\omega = \{t : t \cap \ell_k \neq \varnothing\}$ be a simply connected region in the tiling. We define the continuous bijections

$$\phi^k(x) = \sum_{t \in S^k} \chi(t)(\lambda_t + \phi_t(x)),\ x \in \cup S^k \tag{3.2}$$

Enumerate the tiles above using the same convention as the loop. We define $\phi^k(t_i) := m_i = t_0 + \lambda_i$. In an anti-clockwise fashion, we choose ϕ_t and λ_t so that ϕ is continuous across t_2 and t_1, t_3 and t_2 and so on.

It is impossible to define this bijection in a continuous way when $k = n$. We arrive at two forms of discontinuity when we attempt to make ϕ^n continuous across t_1 and t_n. Depending on where around the defect we started the loop, either $\phi(t_n) = \phi(t_1) = m_1$ or there is a tile m_{n+1} "missing". In both cases, we have that

$$\lim_{x \to \partial t_n^+} \phi_n - \lim_{x \to \partial t_1^-} \phi_1 = e_1,$$

where the $+$ and $-$ denote a line moving with and against the loop ordering respectively. We define the Burgers vector using bijections by

$$e_1 = \sum_{e \in \ell} \Delta \phi_t := \sum_{x_i \text{ endpoints}} \phi_t(x_i) - \phi_t(x_{i-1}) := b_D \in \Lambda,$$

where the x_i are the endpoints of each edge in the contour ℓ ordered anti-clockwise (as the edges in ℓ are). The value of which co-incides with summing edge types around the defect. While the right hand side is always the same value as long as the ϕ_k are continuous, there are many different choices of λ_t. To avoid needing to define λ_t and the regions M^k that ϕ^k maps S^k to, we can instead use the local deformation.

Lemma 3.1.2 (Local Deformation is Locally a Gradient)**.** *For the discontinuous bijection $\phi^n(x)$, the local deformation V^ω defined through a tile gradient*

$$V^\omega(x) := \nabla_t \phi^n(x) := \sum_{t \in T^\omega} \chi(t) \nabla_t \phi_t(x)$$

is such that $\operatorname{curl} V = 0$ *on* $\cup T^\omega$*.*

Proof. It is clear that everywhere on $\cup S^n$, V_n^ω can be written as the gradient of a bijection $\phi^k(x)$ where the first tile in the sum in (3.2) is chosen to be a different tile around the defect. It follows that the vector field is curl free. To extend V_n^ω to a vector field $V^\omega : \cup T^\omega \to \mathbb{R}^{2\times 2}$, we repeat the construction for any overlapping covering of $\cup T^\omega$.

Due to the consistent labelling of the tiling and a fixed set of local bijections, the values that V^ω takes for each such labelling are not sensitive to the choice of starting tile. The different labellings produce $|\Gamma|$ overall choices for V^ω defined on all of $\cup T^\omega$. For each one, the circulation around the defect is a lattice vector and $\operatorname{curl} V^\omega = 0$. $\square$

This gives us a choice of vector field that is defined *globally* on $\cup T^\omega$, not just on local, simply connected regions. Each vector field $V^\omega \in L^2_{loc}(\cup T^\omega, \mathbb{R}^{2\times 2})$ is such that, as above,

$$\oint_{\partial D} V^\omega \cdot dl = \sum_{e \in \ell} \Delta\phi_t = b_D \in \Lambda, \quad \operatorname{curl} V = 0 \text{ in} \cup T^\omega.$$

The above provides this field with useful analytical properties as we will see later. As the above demonstrates, the translational symmetry of the lattice produces defects that make working with displacements (the bijections ϕ and regions of the reference tiling M^k) unwieldy. The vector field V^ω above is defined through a local displacement only but still carries global information about the defects, and (once canonical local bijections are chosen) is unique up to a global rotation for any configuration with a consistent labelling. This object will be the main focus in both analytical and statistical results.

3.1.1 Two Translational Defects: Screening

The discrete rotational symmetry of the lattice means that for each configuration, the value that Burgers vectors take is decided by a specific choice of a rotation from Γ. However, regardless of this choice for each configuration, due to the fact that the labelling when (well-separated) translational defects exist is always consistent, the property that defects can *screen* each other always holds. Considering Figure 2.8, note that the net Burgers vector around the whole configuration is 0, since summing edges around the boundary of the picture yields no net edges. Regarding this as the circulation of a vector field rather than an edge sum allows us to make analytical statements about such configurations.

Definition 3.1.3. *We say that a set of defects D enclosed by a loop ℓ screen each other if the Burgers vector along this loop equals* 0.

This means that in the shaded region T' of Figure 2.8, $V^\omega|_{T'} = \nabla\phi^\omega$ for some vector potential defined on $\cup T'$. This fact has important implications and motivates the definition of screened vector fields, introduced later. We first discuss rotational defects from the point of view of vector fields.

3.2 Rotational Defects And Local Bijections

We now discuss a defect that poses an analytical problem. Figure 1.5 contains a simple configuration that possess a rotational defect. As before, regardless of which convention for labelling the first edge $(1, 2, 3,$ or $4)$ and regardless of which tile we begin with, we find that we cannot upgrade the local labelling to a global labelling. Travelling around a 1-tile thick contour surrounding the defect, we find that the tile labelling becomes rotated by γ. These configurations have no consistent labelling, and we can identify the presence of the rotational defect through this behaviour. Recall that we named this matrix the Frank vector. This exposes the fact that a consistent labelling in a multiply connected tiling T^ω is genuinely a *global* property of the configuration, not a local one.

We now explore this defect using local bijections, and investigate the properties of the vector field V^ω for this configuration. As before we define the family of bijections on simply connected sub-tilings to yield

$$\phi^k(x) = \sum_{t \in S^k} \chi(t) \left(\lambda_t + \gamma_t \phi_t(x) \right)$$

where we must now include which labelling of the local bijection we shall choose. As before, we demand that these are continuous bijections for all $k < n$ as the region is simply connected, and that $\phi^k(x) = \phi^j(x)$ for all $j > k$ and $x \in \cup S^k$. For $k = n$, at the edge e orthogonal to e_1, e_n that links t_1 to t_n we have

$$\lim_{x \to e+} \phi(x) = \gamma \lim_{x \to e^-} \phi(x).$$

Just as before, depending on where around this defect we start we encounter two kinds of discontinuity. If we were to change the rotation of the first tile so that ϕ^n was continuous across tiles n and 1, we would merely move this discontinuity to another tile in the same fashion as for a translational defect. For translational defects, we got around this fact by defining the *local deformation* on T^ω. Before we discuss this idea again we prove some results regarding the Frank vector defined in Section 2.11:

Lemma 3.2.1. *For each labelling there exists exactly one fixed γ with*

$$\sum_{e_j \in \ell} (\gamma \phi^i_{t_j}(e_j), \phi^i_{t_{j+1}}(e_{j+1})) = 1,$$

and it co-incides with the Frank vector.

Proof. This follows from the fact that each ϕ^k is a continuous bijection and the choice of ϕ^1 is fixed. ϕ^k maps edges to edges in the reference configuration, so the above inner products without γ included take the values $1, 0, -1$ since $\phi_t(e^\omega)$ are themselves edges in Λ. It is clear that all the inner products without γ take the value 1 except for the edges attached to tiles n and 1, where these tiles are orthogonal. The inclusion of γ results in 3 possibilities: every inner product equals -1, in which case the condition is not satisfied, or every inner product equals 0 except for the inner product across the inconsistency in tiling. There is only one γ that makes this inner product 1 rather than -1. □

Lemma 3.2.2. *The Frank vector is the same regardless of the labelling and location chosen for the sub-tiling S^1.*

Proof. Since each ϕ^k can be seen as the restriction of some ϕ^j for $j > k$, and because each ϕ^k is continuous, we can represent every possible ϕ_k by fixing a labelling for S_1, then modifying the bijections

$$\phi^k(x) = \sum_{t \in S^k} \chi(t) \left(\lambda_t + \gamma_t \phi_t(x)\right)$$

by a fixed element γ_S to yield

$$\phi^k(x) = \sum_{t \in S^k} \chi(t) \left(\lambda_t + \gamma_S \gamma_t \phi_t(x)\right).$$

where every possible labelling is expressed by changing γ_S to each element of Γ. By definition, then, for any fixed γ

$$\begin{aligned} 1 &= \sum_{e_j \in \ell} (\gamma \phi^i_{t_j}(e_j), \phi^i_{t_{j+1}}(e_{j+1})) = \sum_{e_j \in \ell} (\gamma \gamma_S \gamma_S^T \phi^i_{t_j}(e_j), \phi^i_{t_{j+1}}(e_{j+1})) \\ &= \sum_{e_j \in \ell} (\gamma \gamma_S \phi^i_{t_j}(e_j), \gamma_S \phi^i_{t_{j+1}}(e_{j+1})), \end{aligned}$$

and so both labellings possess the same Frank vector. This vector is unique. Moreover can be seen by inspection that the location of t_1 is irrelevant. The result follows. □

3.3 Non-existence of V^ω for Rotational Defects

We now discuss the problems a Frank vector $\gamma \neq I$ poses from an analytical standpoint. As before, we wish to move from using local descriptions of configurations to a global one, that both encloses information about the defects and has sufficient regularity to analyse easily. We once again use the configuration detailed above in Section 3.2 and use V_S^ω as a candidate object to describe it. We will start by investigating V_S^ω defined on $\cup S^k$:

$$V_S^\omega = \sum_{t \in \cup S^\omega} \nabla_T \phi_t(x)$$

Note that across tiles where ϕ^k is continuous, we can write

$$V_S^\omega = \nabla \phi^k(x),$$

and so everywhere ϕ is continuous, V is locally a gradient field. For a translational defect, even when ϕ^n becomes discontinuous across a cut this is no issue: by taking the gradient in the interior of each tile, we can write V^k as the gradient of a new bijection $\tilde{\phi}^n$ where the discontinuity is moved to be across another tile. However, this does not work for a rotational defect: V^ω defined on $\cup T^\omega$ is not locally a gradient at this point, and is such that $\operatorname{curl} V^\omega \in H^{-1}(\cup T^\omega)$ and supported along a line. This comes from the fact that V does not satisfy an appropriate jump condition as we will now see.

Lemma 3.3.1. *Let n denote the outward normal of the edge perpendicular to the first and last edges in the loop ℓ_n. Denote the region on the side of t_1 by "-" and the region on the side of t_n by "+". There is no $a \in \mathbb{R}^2$ so that*

$$V_+^\omega - V_-^w = a \otimes n, \ \therefore \operatorname{curl} V \neq 0 \ on \ t_1 \cup t_n. \tag{3.3}$$

where $V_\pm^\omega$ is the value of the deformation field taken as a limit to either side of n.

Proof. A standard result, referred to as the kinematic compatibility condition or Hadamard jump condition (Ball [2004]), yields that for a continuous map ϕ to exist across two sides of an interface that the gradient on either side must satisfy the condition (3.3). As discussed in the previous section, due to the inconsistent labelling we have for some $\gamma \in \Gamma, \gamma \neq I$ and $a \in \mathbb{R}^2$ that

$$V_+^\omega - \gamma V_-^w = a' \otimes n$$

and so

$$V_+^\omega - V_-^w + (\gamma V_-^w - \gamma V_-^w) = a' \otimes n + (\gamma - I) V_-^\omega.$$

It is clear by testing with vectors perpendicular to n that the rightmost term cannot be written in the form $b \otimes n$. Calling $c := V_n^\omega n^\perp$ we require that

$$c^\perp - c = (b \otimes n)n^\perp = 0,$$

but since this is impossible unless $c = 0$ we find the non-existence of the required a in (3.3). $\square$

As discussed above the failure for this jump condition to be satisfied cannot be removed: attempting to 'flip' values merely moves it somewhere else. Therefore, there is no single-valued choice of V^ω so that the globally defined vector field is locally a gradient everywhere on $\cup T^\omega$. These defects produce technical difficulties from an analytical standpoint and generalisations of those results will be discussed separately. We now make some remarks on extensions of the local deformation field from $\cup T^\omega$ to the defect region D^ω.

3.4 Extension of a Local Deformation Field

To avoid using analytical estimates on the domain $\cup T^\omega$, which would result in different rigidity constants for different ω, it is helpful to extend the vector field to all of U_n. This allows us to use the same rigidity constant for all admissible ω for a fixed n.

Lemma 3.4.1 (Extension Into The Defects). *Let $\omega \in \Omega_n$ be an admissible configuration. For all n, there exists an extension $\tilde{V}^\omega : U_n \to \mathbb{R}^{2\times 2}$ such that $\tilde{V}^\omega = V^\omega$ on $\cup T^\omega$, and*

$$|\tilde{V}^\omega| < M_1, \;\; \operatorname{supp} \operatorname{curl} V = (\cup T^\omega)^c, \; |\operatorname{curl} \tilde{V}^\omega| < M_2$$

where M_1, M_2 do not depend on n for large enough n. They instead depend on the other tiling parameters and its regularity constant ρ.

See Aumann [2015] for an elementary construction or use a general extension principle for Lipschitz domains.

In Chapter 5 we will discuss admissible and screened configurations from the point of view of vector fields. These are configurations that have a consistent labelling. This assures that we can globally define the local deformation field V^ω, with the required regularity. We can define a class of vector fields based on these configurations and generalise it to a continuum setting, allowing us to produce rigidity estimates that are more suitable to use as tools in statistical mechanics than current ones in the literature. We will also treat vector fields with rotational defects from an analytical standpoint with a generalised rigidity estimate proved in Chapter 4, but we are unable to rigorously demonstrate ordering results in a statistical sense for configurations that possess these defects. However, we can produce results regarding the expectation of the energy when they are included in such a system.

Chapter 4

Rigidity for Curl-Free & Symmetrisable Vector Fields

4.1 Rigidity for Gradient Vector Fields: Review

In order to avoid some of the notation from the previous section, we will work with a simplified framework, and reduce to the special case of vector fields needed in the statistical mechanics section. The goal of this chapter is to adapt the geometric rigidity estimate found in Friesecke et al. [2002]:

$$\exists R \in \mathrm{SO}(2) : \|\nabla u - R\|_{L^2(U_n)} \leq C_{RIG}(U_1)\|\mathrm{dist}(\nabla u, \mathrm{SO}(2))\|_{L^2(U_n)}, \tag{4.1}$$

where $C_{RIG}(U_1)$ is scale-invariant and depends on the Lipschitz constant of U_1, to a large class of vector fields $V \in L^2(U_n, \mathbb{R}^{2\times 2})$. In two dimensions, it has been found that $C_{RIG} = \sqrt{2}$ for $U_1 = [0,1]^2$ in Lewicka and Müller [2015]. For some simply connected, bounded set U and $r \geq 0$ we work with vector fields

$$A_r(U_n) = \{V \in L^2_{\mathrm{curl}}(U) : \ \mathrm{supp}\,\mathrm{curl}\,V \subset \cup_i^M B_r(x_i) : \text{for disjoint } (B(x_i))_{i=1}^M.\}$$

We are particularly interested in the form of the rigidity estimate for large n, as this has implications in the statistical mechanical model we will consider.

4.2 Rigidity for Curl-Free Vector Fields

Theorem 4.2.1 (Rigidity for Curl-Free Vector Fields)**.** *Let Let U be a Lipschitz domain, not necessarily simply connected. Let $V \in L^2(U)$ be such that* $\mathrm{curl}\,V = 0$

a.e. in U. Then for any such V there exists a fixed rotation $R \in \mathrm{SO}(2)$ such that

$$\|V - R\|_{L^2(U)} \leq C_{RIG} \|\mathrm{dist}(V, \mathrm{SO}(2))\|_{L^2(U)},$$

where the constant above is the rigidity constant found in Equation 1.1.

Proof. We follow the arguments for the original rigidity estimate found in Friesecke et al. [2002], but modify the statements when appropriate. It is assumed WLOG that the vector field $V : |V|_\infty \leq C(M)$ for some constant M dependent only on the dimension.

We will show that for every curl-free, square-summable vector field that there exists a curl-free vector field $W : |W|_\infty \leq C(M)$ with the property that

$$\|V - W\|_{L^2(U)} \leq C(U) \|\mathrm{dist}(V, \mathrm{SO}(2))\|^2_{L^2(U)} \tag{4.2}$$

where $C(U)$ depends only on the Lipschitz constant of the domain. Should this vector field exist, and should there exist a constant rotation so that for all vector fields $W : |W|_\infty < C(M)$

$$\|W - R\|_{L^2(U)} \leq C \|\mathrm{dist}(W, \mathrm{SO}(2))\|_{L^2(U)},$$

the claim is established by a simple application of the triangle inequality and employing Equation 4.2. When $V = \nabla v$ for some $v \in H^1(U, \mathbb{R}^2)$, Lemma A.1 of Friesecke et al. [2002] yields the existence of a function

$$u : U \to \mathbb{R}^2, \;\; |\nabla u| \leq C(M),$$

and

$$\|\nabla v - \nabla u\|_{L^2(U)} \leq C(U) \|\mathrm{dist}(\nabla v, \mathrm{SO}(2))\|_{L^2(U)}$$

(For a proof see Friesecke et al. [2002]). Using the approximation theorem, the claim in Equation (4.2) is proved for gradients. As we have a curl-free vector field V, we will take our Lipschitz domain U and cover it with a family of simply connected, Lipschitz subdomains $\{U_i\}_{i \geq 1}$. Because our vector field V is curl-free, $V = \nabla v_i$ on each U_i. We will apply this approximation theorem to each simply connected subdomain U_i and the restriction of V to that subdomain. This gives us the family of maps u_i each supported on U_i such that

$$\|V - \nabla u_i\|_{L^2(U_i)} \leq C(U_i) \|\mathrm{dist}(V, \mathrm{SO}(2))\|_{L^2(U_i)}$$

We must now use these u_i to construct a curl free vector field W that obeys the needed inequality. To this end write that $V = \nabla v_i$ on each U_i. Now, let ϕ be a partition of unity subordinate to U_i in which we assume each U_i is simply connected. We define the vector field

$$W = \sum_i \nabla(\phi_i u_i), \quad \Longrightarrow \operatorname{curl} W = 0.$$

Note that on each U_k

$$\int_{U_k} |V - W|^2 = \int_{U_k} |\sum_i \nabla\phi_i u_i + \phi_i \nabla u_i - \sum_i \phi_i \nabla v_k|^2 \tag{4.3}$$

using $\sum_i \phi_i = 1$. We then have

$$\int_{U_k} |V - W|^2 \leq \left\| \sum_i \phi_i (\nabla u_i - \nabla v_k) \right\|^2_{L^2(U_k)} + \int_{U_k} |\sum_i \nabla \phi_i u_i|^2$$

we consider the rightmost term separately. Take

$$\sum_i \nabla\phi_i u_i = \sum_{j: v_k = u_j} \nabla\phi_j v_k + \sum_{i: v_k \neq u_i} \nabla \phi_i v_k - \sum_{i: v_k \neq u_i} \nabla\phi_i v_k + \sum_{j: v_k \neq u_j} \nabla \phi_j u_j,$$

$$\sum_i \nabla\phi_i u_i = \sum_i \nabla\phi_i v_k - \sum_{i: v_k \neq u_i} \nabla\phi_i v_k + \sum_{j: v_k \neq u_j} \nabla\phi_j u_j = 0 + \sum_{i: v_k \neq u_i} \nabla\phi_i (u_i - v_k). \tag{4.4}$$

A result in the proof of Proposition 3.1 of Friesecke et al. [2002] yields, for all $V : |V|_\infty > C(M)$ that on each U_k

$$\| \sum_{i: v_k \neq u_i} \nabla(u_i - v_k)\|^2_{L^2(U_i)} \leq C(U_i) \int_{\nabla v_k \geq C(M)} |\nabla v_k|^2 \leq C \|\operatorname{dist}(\nabla v_k, \mathrm{SO}(2))\|^2_{L^2(U_k)} \tag{4.5}$$

As in the proof of Theorem 3.1 in Friesecke et al. [2002] the above only depends on the Lipschitz constant of the domain. All that remains is to extract the term $\nabla\phi_i$. Applying an L^∞ estimate for the partition which generates a constant depending on the Lipschitz constant of U_i, the Poincaré inequality to the rightmost term of Equation (4.4) (As we only deal with gradients we can choose potentials with mean zero), and the estimate Equation (4.5) to the result, we arrive at a vector field W such that $|W|_\infty < M$ and

$$\|V - W\|_{L^2(U)} \leq C(U) \|\operatorname{dist}(V, \mathrm{SO}(2))\|_{L^2(U)},$$

where C depends on the Lipschitz constant of U, upon recalling Equation (4.3). Without loss of generality, then, we also assume that $|V|_\infty \leq C(M)$ in the following.

Lemma 4.2.2. *Let $Q \subset \mathbb{R}^2$ be a cube and let Q' be a concentric one with half the width. Then for all curl-free vector fields V there exists a rotation R_Q with*

$$\|V - R_Q\|_{L^2(Q)} \leq C\|\mathrm{dist}(V, \mathrm{SO}(2))\|_{L^2(2Q)}.$$

For a proof see Friesecke et al. [2002], using the fact that curl-free vector fields on simply connected regions can be expressed as gradients. We now recount an argument from Friesecke et al. [2002] regarding the decomposition above. Since V can be written as a gradient on any simply connected region, we find that pointwise, just as in Friesecke et al. [2002] that

$$\mathrm{div}\ \mathrm{cof}V = 0,\ \mathrm{div}V = \mathrm{div}(V - \mathrm{cof}V).$$

(See 8.1 Evans [1998]) As in Friesecke et al. [2002] and demonstrated above using a similar method, assuming WLOG that $|V|_\infty \leq C(M)$ there exists an absolute constant that does not depend on U so that

$$|\mathrm{cof}V - V| \leq C|\mathrm{dist}(V, \mathrm{SO}(2))|.$$

We now introduce the decomposition

$$\begin{cases} -\Delta z = \mathrm{div}V, \\ z \in H_0^1(U) \end{cases}$$

(See Evans [1998]) and take $W := V - \nabla z$. Applying the above, we find

$$\int_U |\nabla z|^2 \leq \int_U |V - \mathrm{cof}V|^2 \leq C\|\mathrm{dist}(V, \mathrm{SO}(2))\|_{L^2(U)}^2.$$

It remains to show there exists a rotation R_U with

$$\|W - R_U\|_{L^2(U)}^2 \leq C\|\mathrm{dist}(V, \mathrm{SO}(2))\|_{L^2(U)}^2.$$

Assuming this claim is true, we note that combining the above yields

$$\begin{aligned} \|V - R\|_{L^2(U)} &\leq \|W - R\|_{L^2(U)} + \|\nabla z\|_{L^2(U)} \leq C\|\mathrm{dist}(V - \nabla z, \mathrm{SO}(2))\|_{L^2(U)} + \|\nabla z\|_{L^2(U)} \\ &\leq C(U)\|\mathrm{dist}(V, \mathrm{SO}(2))\|_{L^2(U)}. \end{aligned}$$

The claim is demonstrated by making minor modifications to work in Friesecke et al. [2002]. We must work with an appropriately constructed curl-free vector field rather than a gradient. We must use the previously constructed objects that are now curl-free vector fields rather than gradients. This allows us to apply the rigidity estimate to general Lipschitz domains rather than cubes for curl-free vector fields, with a rigidity constant that has the same behaviour as $C_{RIG}(U_1)$. To quantify the rigidity constant in certain cases we must examine a variant of the Poincaré inequality on discs with a small hole.

To point out the behaviour of the rigidity constant and these modifications we reproduce the relevant parts of the proof. To this end, we write $Q_i = a + r_i(-1,1)^2$. We exhaust U by cubes Q_i such that $\sum_i \chi(Q_i) \leq N$ for some fixed $N \in \mathbb{N}$, such that

$$2r_i \leq \operatorname{dist}(a_i, \partial Q_i) \leq Cr_i.$$

Since $\operatorname{curl} W = 0$ we may apply the rigidity estimate for cubes to yield

$$\int_{Q_{2r_i}} |W - R_i|^2 \leq \int_{Q_{4r_i}} |\operatorname{dist}(W, \mathrm{SO}(2))|^2.$$

Noting W is divergence free by definition, on each cube $Q(a_i, 4r_i)$ W can be written as the gradient of a harmonic potential w_i and so is also harmonic. Because of this fact, as in Friesecke et al. [2002] we may apply Caccioppoli's inequality to yield

$$r_i^2 \int_{Q_{r_i}} |\nabla W|^2 \leq C \int_{Q_{2r_i}} |W - R_i|^2.$$

where the right hand side is a curl-free vector field rather than a gradient as in Friesecke et al. [2002]. We can sum over cubes to produce a global inequality that depends on the covering, but not the domain. We now state two results that come from the proof of the rigidity theorem from Friesecke et al. [2002] and the corollary above:

Lemma 4.2.3. *There exists an absolute constant (but depending on N) such that*

$$\int_U \operatorname{dist}(x, \partial U) |\nabla W|^2 \leq C \int_U |\operatorname{dist}(W, \mathrm{SO}(2))|^2.$$

Lemma 4.2.4. *It can be shown that for some scale-invariant C depending on the domain that*

$$\min_{R \in \mathrm{SO}(2)} \|W - R\|^2_{L^2(U)} \leq C \int_U |\nabla W|^2 |\operatorname{dist}(x, \partial U)|^2 \tag{4.6}$$

by applying both a weighted Sobolev and ordinary Poincarè inequality.

Both of which come from Friesecke et al. [2002]. The first is evident from the properties of the covering above. From these lemmas the claim is immediate, recalling that the right hand side of (4.6) is the left hand side of the term in Lemma 4.2.3. □

The reason we state the lemmas above is that for later results, it is important to know the behaviour of the rigidity constant for a class of punctured domains. The behaviour of these constants allows us to generalise results in the statistical mechanics chapter further by introducing dipoles of unbounded length.

4.3 Sobolev Estimates for Punctured Domains

We begin this section proving some properties of the estimates that underpin the rigidity estimate for gradients and curl-free vector fields.

4.3.1 Weighted Sobolev Estimates, Annuli and Scaling

Lemma 4.3.1 (Scaling of the WSE). *For a Lipschitz domain $U \subset \mathbb{R}^2$, write the weighted Sobolev estimate as*

$$\int_U |g|^2 dx \leq C_1 \int_U |g|^2 \mathrm{dist}(x, \partial U)^2 dx + C_2 \int |\nabla g|^2 \mathrm{dist}(x, \partial U)^2 dx.$$

It is such that for all $\eta > 1$, we can take $C_2(\eta U) = C(U)$, $C_1(\eta U) = \eta^{-2}$.

Proof. For the theorem itself see Theorem 1.5 of Nečas [1962]. To establish this we use a scaling argument. Let U be some Lipschitz domain and take $\tilde{U} = \eta U$. Let $\tilde{g} \in L^2(\eta U)$. We define $g(x) = \tilde{g}(\eta x)$ for $x \in U$ and assume $\eta \geq 1$. With this we find

$$\int |g(x)|^2 = \eta^{-2} \int_{\tilde{U}} |g(y)|^2 dy.$$

We have that

$$\nabla_x g(x) = n \nabla_y \tilde{g}(y), \;\; |\mathrm{dist}(x, \partial U)|^2 = \eta^{-2} |\mathrm{dist}(y, \partial \eta U)|^2.$$

From these we find

$$\int_U |g|^2 |\mathrm{dist}(x, \partial U)|^2 = \eta^{-4} \int_{\tilde{U}} |\tilde{g}|^2 |\mathrm{dist}(y, \partial \eta U)|^2 dy,$$

$$\int_U |\nabla g|^2 |\mathrm{dist}(x,\partial U)|^2 = \int_{\tilde{U}} \eta^2 |\nabla \tilde{g}|^2 \eta^{-2} |\mathrm{dist}(y,\partial \eta U)|^2 \eta^{-2} dy$$
$$= \eta^{-2} \int_{\tilde{U}} |\nabla \tilde{g}|^2 |\mathrm{dist}(y,\partial \eta U)|^2 dy.$$

It follows that upon application of the WSE

$$\int_{\tilde{U}} |g|^2 = \eta^2 \int_U |g|^2 \le \eta^{-2} C_1 \int_{\tilde{U}} |\tilde{g}|^2 \mathrm{dist}(y,\partial \eta U) dy + C_2 \int_{\tilde{U}} + |\nabla \tilde{g}|^2 \mathrm{dist}(y,\partial \eta U) dy.$$

□

Corollary 4.3.2. *Note that for the regular Poincaré inequality the above yields for some $a \in \mathbb{R}$ that*

$$\int_{\eta U} |g-a|^2 \le \eta^{-2} C(U) \int_{\eta U} |\nabla g|^2 dx$$

by using the same calculations as in the start of the above proof, the inequality itself can be found for instance in Lieb and Loss [2001].

These considerations lead to the following results for weighted Sobolev and rigidity estimates on punctured discs.

Lemma 4.3.3 (Weighted Sobolev Estimates for the Punctured disc)**.** *Let $U = B_1(0)$ and let $0 < \epsilon < 1/2$. Define $U_\epsilon = B_1(0) \backslash B_{\epsilon(0)}$. For all $g \in L^2(U_\epsilon) \cap H^1_{loc}(U_\epsilon)$ we have*

$$\int_{U_\epsilon} |g|^2 dx \le C_1 \epsilon^{-2} \int_{U_\epsilon} |g|^2 \mathrm{dist}(x,\partial U)^2 + C_2 \int_{U_\epsilon} |\nabla g|^2 \mathrm{dist}(x,\partial U)^2 dx,$$

where C_1, C_2 do not depend on ϵ.

Corollary 4.3.4. *The same holds for the Poincaré inequality on the annulus,*

$$\int_{U_\epsilon} |g-a|^2 \le C_p(B_2 \backslash B_1) \epsilon^{-2} \int |\nabla g|^2 dx.$$

Proof. To show this we apply the inequality to the family of annuli $A_k = B_{(k+1)\epsilon} \backslash B_{k\epsilon}$ for $k \ge 1$. Consider $k = 1, k = 2$ to begin with. Since the second term on the right hand side plays no role in this estimate we write it as $I_2(X)$ where X is the set whose boundary is used in the dist term.

$$\int_{A_1} |g|^2 dx \le C(B_2 \backslash B_1) \epsilon^{-2} \int_{A_1} |g|^2 \mathrm{dist}(x,\partial A_1)^2 + I_2(A_1)$$
$$\le C(B_2 \backslash B_1) \epsilon^{-2} \int_{A_1} |g|^2 \mathrm{dist}(x,\partial U_\epsilon)^2 + I_2(U_\epsilon)$$

We now apply this inequality to the domain A_2 and the restriction of g to this domain. The inequality possesses the same constants. Putting these together yields

$$\int_{A_1\cup A_2}|g|^2dx \le C(B_2\backslash B_1)\epsilon^{-2}\int_{A_1\cup A_2}|g|^2\text{dist}(x,\partial U_\epsilon)^2 + C_2\int_{A_1\cup A_2}|\nabla g|^2\text{dist}(x,\partial U_\epsilon)^2,$$

since the annuli are disjoint. We repeat this procedure until we reach the desired outer radius of the annulus U_ϵ. The above can be used for the regular Poincaré inequality using the same decomposition. □

4.4 The Rigidity Constant for a Punctured Domain

Theorem 4.4.1. *[Rigidity for Curl-Free Vector Fields in a Punctured Domain] Let $U = B_r(0)$ for $r \ge 1$, and let $0 < \epsilon < 1/2$. As before, define the punctured domains $U(\epsilon, r) = B_r(0)\backslash B_{\epsilon(0)}$. Then for all $V \in L^2(U(\epsilon, r), \mathbb{R}^{2\times 2})$ with $\operatorname{curl} V = 0$ in $U(\epsilon, r)$) there exists a fixed rotation $R \in \mathrm{SO}(2)$ such that*

$$\|V - R\|_{L^2(U(\epsilon,r))} \le C(B_2\backslash B_1)\|\text{dist}(V, \mathrm{SO}(2))\|_{L^2(U(\epsilon,r))}.$$

That is, we may take the constant to be uniform on the family of domains $U(n, \epsilon_0)$ for some fixed ϵ_0 and all $n \in \mathbb{N}$.

Proof. This is a direct consequence of the lemmas established above. We follow the proof of Theorem 3.1 in Friesecke et al. [2002] using the estimates above. We first work with the domain $U(1, \epsilon)$ for fixed ϵ. Recall the WSE for the annulus $U_\epsilon := U(\epsilon, 1)$

$$\int_{U_\epsilon}|g|^2dx \le \epsilon^{-2}C_1\int_{U_\epsilon}|g|^2\text{dist}(x,\partial U_\epsilon)^2 + C_2\int|\nabla g|^2\text{dist}(x,\partial U_\epsilon)dx.$$

Fix $\delta : \delta^2\epsilon^{-2}C_1 \le 1/2$ and define the set $q_\delta = \{x : \text{dist}(x, \partial U_\epsilon) \ge \delta\}$. In this case, again $q_\delta = CU(\epsilon, r)$ where the constant is some scale-invariant factor since $\delta \lesssim \epsilon$. Denoting by C_q the constant for the ordinary Poincaré inequality on $B_2\backslash B_1$, for this annulus Corollary 4.3.4 yields for any f the existence of some $a \in \mathbb{R}^2$ with

$$\int_{q_\delta}|f-a|^2 \le C_p\epsilon^{-2}\int_{q_\delta}|\nabla f|^2dx.$$

We will estimate $f-a$ on the whole of U_ϵ as in Friesecke et al. [2002]. Applying the WSE to $g := f-a$ on $U_\epsilon \backslash q_\delta$, and noting that $\mathrm{dist}(x, \partial U_\epsilon)\epsilon^{-2}C_1 \leq \frac{1}{2}$ on $U\backslash q_\delta$ yields

$$\int_{U_\epsilon \backslash q_\delta} |f-a| \leq \frac{1}{2}\int_{U\backslash q_\delta} |f-a|^2 + C_2 \int_{U_\epsilon \backslash q_\delta} |\mathrm{dist}(x,\partial U_\epsilon)|^2 |\nabla f|^2 dx. \tag{4.7}$$

Moving the first term on the right hand side gives us the result required up to a constant. On q_δ we find

$$\frac{1}{2}\int_{q_\delta} |f-a|^2 \leq C_p \epsilon^{-2} \int_{q_\delta} |\nabla f|^2 dx \leq C\frac{\epsilon^{-2}}{\delta^2}\int_{q_\delta} |\nabla f|^2 \mathrm{dist}(x,\partial U_\epsilon)^2.$$

As we can fix $\delta \propto \epsilon$ we may take some overall constant (Noting $U\backslash q_\delta$ is a union of annuli), not depending on ϵ, so that

$$\int_{U_\epsilon \backslash q_\delta} |f-a|^2 \leq C(B_2\backslash B_1)\int_{U_\epsilon \backslash q_\delta} |\nabla f|^2 \mathrm{dist}(x,\partial U_\epsilon)^2. \tag{4.8}$$

We can estimate the norm of $f-a$ on U_ϵ by applying (4.8) to q_δ and the WSE (4.7) to its complement. Combining the above yields

$$\int_{U_\epsilon} |f-a| \leq (C(B_2\backslash B_1) + C_2(B_2\backslash B_1))\int_{U_\epsilon} |\mathrm{dist}(x,\partial U_\epsilon)|^2 |\nabla f|^2 dx.$$

Applying this component wise to the entries of ∇W where W is the curl- and divergence-free part of V as in (4.6), and noting these elements a_{ij} can be chosen to lie in SO(2) by considerations in Friesecke et al. [2002] yields

$$\min_{R\in \mathrm{SO}(2)} \|W-R\|^2_{L^2(U_\epsilon)} \leq C(B_2\backslash B_1)\int_{U_\epsilon} |\nabla W|^2 |\mathrm{dist}(x,\partial U_\epsilon)|^2.$$

Since this constant is scale invariant, we choose for $\epsilon' = \mathrm{diam}(U_\epsilon)^{-1}\epsilon$ the domain $U(\epsilon', 1)$ and rescale to arrive at the estimate for domains $U(\epsilon, r)$. This establishes (4.4.1) for vector fields $|V|_\infty \leq C(M)$. To move to the full rigidity estimate, we must show that the Lipschitz constant of this domain is invariant when it comes to ϵ. Since the boundary is composed of two balls, both of whose Lipschitz constants can be chosen to be a constant proportional to 1 by rescaling, the proof is finished. □

4.5 Symmetrised Vector Fields

We now introduce a generalisation to the above setting in which the vector field V cannot locally be written as a gradient everywhere, inspired by the considerations made to rotational defects in Chapter 2. We establish what is means to symmetrise a vector field $V \in L^2_{loc}(\mathbb{R}^2)$ with respect to a discrete group Γ, generalise a notion of curl to this space of symmetrised fields, and prove a rigidity estimate for vector fields that are (in a generalised sense) curl-free on a not necessarily simply connected domain. As before, the constant obtained will be scale invariant, but due to the lack of an extension theorem for these objects the rigidity estimate cannot currently be used in the same way as others. Nonetheless, we will use the generalised rigidity estimate to give a heuristic argument that "large" disclinations in isolation are not expected at finite temperature in the model introduced in Chapter 6. However, discussion of vector fields possessing both translational and rotational defects is currently limited.

4.5.1 Vector Fields and Rotational Symmetry

As before, for concreteness we work with the square lattice $\mathbb{Z}^2$ and the rotational symmetry group Γ of t_0. Recall that in Chapter 3, Subsection 3.03, we took a restricted tiling S^ω such that the continuum domain $\cup S^\omega$ was simply connected. We defined the local deformation

$$V_S^\omega(x) = \sum_{t \in S^\omega} \gamma_t \nabla_t \phi_t(x)$$

where ϕ_t map tiles to the reference tile and γ_t are some arbitrary rotations from the symmetry group of $\mathbb{Z}^2$. We wish to choose the γ_t so that $\operatorname{curl} V_S^\omega$ exists as a function and is equal to 0 on the tiling. As previously mentioned, we can make such choices when the tiling has a consistent labelling. A simply connected restricted tiling always has this labelling. If $\cup S^\omega$ is multiply connected, these choices of γ_t can be impossible even if S^ω is a restricted tiling. That is, we will always end up with a measure-valued curl somewhere in the domain $\cup S^\omega$ when evaluating $\operatorname{curl} V_S^\omega$. To do away with some notation concerning tilings, we will now introduce a continuum analogue of the local deformation with no underlying length scale (enforced by the length of a tile). We can then discuss the regularity of some appropriate vector fields in a more abstract way. All the results will apply to candidate local deformations for tilings that we define.

Definition 4.5.1. *Let U be a Lipschitz domain. We say a vector field $V \in L^2(U)$ can be symmetrised with respect to a lattice Λ if, for any simply connected domain $S \subset U$, there exists a function $\gamma \in L^2(S, \Gamma)$ such that*

$$\operatorname{curl}(\gamma V) = 0, \quad \textit{on } S.$$

We say $V \in L^2_{sym}(U;\Gamma)$ and say $\mathrm{Curl} V = 0$.

In addition to these, we define the symmetrised rotations which use a globally defined vector field γ:

Definition 4.5.2 (Symmetrised Rotations)**.** *Let $R \in SO(2)$ and let $\gamma \in L^2(U,\Gamma)$. We say a symmetrisation of R is the vector field $\gamma(x)R$ for any $\gamma \in L^2(U,\Gamma)$. We call the space of all symmetrised rotations in a domain U as*

$$\underline{R} \in \mathrm{SO}(2)_\Gamma(U) \text{ if } \underline{R}(x) = R\gamma(x) \text{ for all } x \in U$$

where $R \in \mathrm{SO}(2)$ is fixed for each $\underline{R}$ for all x and $\gamma \in L^2(U,\Gamma)$.

We first present a lemma that is a corollary of the geometric rigidity estimate for gradient fields, and then proceed to generalise it to include the case of disclinations.

Lemma 4.5.3. *Let U be a simply connected, Lipschitz domain. For any $V \in L^2_{sym}(U;\Gamma)$ there exists a rotation $R \in \mathrm{SO}(2)$ and $\gamma \in L^2(U,\gamma)$ such that*

$$\|V - \gamma R\|_{L^2(U)} \leq C(U)\|\mathrm{dist}(V, \mathrm{SO}(2))\|_{L^2(U)}.$$

Proof. Since U is simply connected, as noted above for some potential $\varphi \in H^1(U,\mathbb{R}^2)$ we have $\gamma V = \nabla\varphi$. Applying the rigidity estimate to the latter object we find

$$\|\nabla\varphi - R\|_{L^2(U)} = \|V - \gamma(x)^T R\|_{L^2(U)} \leq C\|\mathrm{dist}(V, \mathrm{SO}(2))\|_{L^2(U)}.$$

Since γ is pointwise a rotation, so is γ^T and the claim follows. $\square$

We now establish a condition on whether or not we can symmetrise a vector field on multiply connected set. Whether or not this is trivial is of course related to whether or not the vector field possesses a non-trivial Frank vector.

Lemma 4.5.4. *Let U be a Lipschitz domain with a single hole and let $V \in L^2_{sym}(U)$ have a non-trivial Frank vector: that is there exists a unique line ℓ such that*

$$V_+ - \gamma_F V_- = a \otimes n, \quad \mathrm{curl}\, V = 0 \text{ on } U \backslash \ell$$

for some fixed $\gamma_F \neq I$, and $\pm$ denotes the limit of V on either side of this line. Then there is no choice of $\gamma \in L^2(U,\Gamma)$ such that $\mathrm{curl}\,\gamma V = 0$ *on U.*

To demonstrate this we require another lemma.

Lemma 4.5.5. *Suppose that on some simply connected set that $\gamma(x)V(x) = \nabla u(x)$. Then the only other choices γ' so that $\gamma' V = \nabla u'$ are global rotations γ_G of γ.*

Proof. Suppose there exists a function u with $\nabla u = \gamma_1 V$ and let $\beta = \gamma_2 V$. Let $\gamma' = \gamma_2 \gamma_1^T$ and consider

$$\beta = \gamma' \nabla u_1 = \nabla(\gamma' u) - u \otimes \mathrm{div}\gamma'$$

and so the only way β itself is a gradient is if γ' is constant. □

Proof of Lemma 4.5.4. The proof uses the same idea as in the discussion of rotational defects in locally lattice-like domains. Pick a set $U_1, \ldots, U_n$ of simply connected domains so that $\cup U_n = U$ and U_n are disjoint, and say $\ell \subset \partial U_1$. Define

$$V_n = \sum_{k=1}^{n} \chi(U_k)\gamma_k V, \quad \mathrm{curl}\, V_n = 0$$

We know that on $\cup S_k \backslash \ell$ there is, up to a global rotation γ_G, a single choice $\gamma(x)$ such that $\mathrm{curl}\, \gamma(x)V = 0$. In the above the $\gamma_k(x)$ are restrictions of this $\gamma(x)$, potentially multiplied by the fixed rotation matrices γ_k on S_k. However, this vector field is not rank-one connected across ℓ: modifying it to be across ℓ involves a global rotation of V_1 by a constant rotation γ_G. In order for V_2 to be a gradient we must propagate this rotation so that $\gamma_2 = \gamma_G \gamma_k \gamma(x)|_{x \in S_k}$. Continuing in this way, we again arrive at a vector field with the same Frank vector as before. The Frank vector persists, with V merely being globally rotated by an element of the symmetry group. □

To establish a rigidity estimate for these fields, we follow the methods of the proof in Aumann [2015], with modifications that reflect the fact that V can fail to be rank-one connected in the domain. We believe that it is informative to give a proof of this in the framework locally lattice-like tilings and the deformation field, as well as a general analytical one. This serves to show why care was taken in establishing notation around the discrete symmetries of the lattice and local bijections. With these estimates in place, we return to symmetrisable vector fields in the next chapter, to present a combined rigidity estimate for vector fields with translational and rotational defects.

4.6 Rigidity for Symmetrised Vector Fields

We now return to configurations like the one demonstrated in 3.3 that do not have a consistent, global labelling of edges in T^ω but are otherwise free of defects. For these fields we will provide a rigidity estimate that depends on the domain $\cup T^\omega$.

4.6.1 Symmetrised Deformation Fields

Definition 4.6.1 (Symmetric Local Deformation). *Let $\omega \subset U$ be a finite subset of a Lipschitz domain U. Let T^ω be the tiling as obtained in Chapter 2. Let v_t be some canonical choice of continuous bijections for each tile into $t_0 = [0,1]^2$. For each tile $t \in T^\omega$ let ∇v_t^i, $i \in \{1,..,4\}$ be the local deformations associated with it. We define the collection of local deformations at a point x to be*

$$V^i(x) = \nabla v_t^i(x), \text{ if } x \in t.$$

On any simply connected region S^ω there exists a collection $\{i(t)\}_{t\in S^\omega} \in \{1,2,3,4\}^{|S^\omega|}$ such that $\operatorname{curl} V^{i(t)} = 0$ on $\cup S^\omega$. That is, for an arbitrary choice of $i(t) : t \in T^\omega$, we can find a vector field $V^\omega \in L^2_{sym}(\cup T^\omega)$ that represents the local deformation of the configuration by taking $V^\omega(x) = V^{i(t)}(x), x \in \cup T^\omega$. We call $V^\omega \in L^2_{sym}(\cup T^\omega, \mathbb{R}^{2\times 2})$ a symmetrised local deformation field of T^ω.

V^ω is the global object that we can work with for inconsistently oriented configurations- while as discussed it is impossible to define a single-valued field with the right regularity globally, we can use any one of these objects and a generalised notion of curl to store global information about defects and recover the required regularity properties on simply connected regions.

4.6.2 Geometric Rigidity for Symmetrised Vector Fields

Theorem 4.6.2. *Let U be a Lipschitz domain, $\omega \subset U$ a finite set and T^ω the locally lattice-like tiling associated to it. Let V^ω be a symmetric vector field associated with it and recall $\operatorname{Curl} V^\omega = 0$ on $\cup T^\omega$. For each such V^ω there exists a constant rotation $R^\omega \in \mathrm{SO}(2)$ and some $\gamma^\omega \in L^2(\cup T^\omega, \Gamma)$ such that*

$$\|V^\omega - \gamma^\omega R^\omega\|_{L^2(\cup T^\omega)} \leq C(\cup T^\omega)\|\operatorname{dist}(V^\omega, \mathrm{SO}(2))\|_{L^2(\cup T^\omega)}.$$

In fact, for any Lipschitz domain U and any vector field $V \in L^2_{sym}(U;\Gamma)$ there exists some $\gamma \in L^2(U,\Gamma)$ and some $R \in \mathrm{SO}(2)$ with

$$\|V - \gamma R\|_{L^2(U)} \leq C(U)\|\mathrm{dist}(V, \mathrm{SO}(2))\|_{L^2(U)}.$$

In both cases, the constant is scale invariant.

Proof. The proof proceeds in a similar way to Aumann [2015] for curl-free fields and we follow the method therein, with some technical difficulties. Recall that T^ω is locally lattice like and that simply connected, overlapping sets $S_1, ..., S_J$ can be constructed. We can pick appropriate values of $\gamma_i(x), i \leq J$ defined on S_j so that $\gamma_j V^\omega$ is a gradient on each region. Suppose WLOG that T^ω can be split into two simply connected regions S_1, S_2.

This implies that we can collect a set $\{i(t)\}_{t \in S_j}$ such that the components $V_j^{i(t)}$ can be expressed as the gradient of some vector field v_j defined on S_j. Note that for some rotation $\gamma \in \Gamma$, not necessarily the identity, that $\gamma_1\phi_1 - \phi_2 = \mathrm{const}$ on $S_1 \cap S_2$ i.e. the two local deformations are not necessarily rank-one connected for locally lattice-like configurations. Geometric Rigidity for vector fields yields the existence of R_1, R_2 such that

$$\|\nabla\phi_j - R_j\|_{L^2(\cup S_j)} \leq \|\mathrm{dist}(\nabla\phi_j, \mathrm{SO}(2))\|_{L^2(\cup S_j)},\ j \in \{1, 2\}.$$

Note that for an arbitrary $\gamma \in L^2(\cup S_j, \Gamma)$

$$\|V - \gamma R_1\|_{L^2(\cup T_2)} \leq \|\nabla v_2 - \gamma R_1\|_{L^2(\cup T_2)} \leq \|\nabla v_2 - R_2\|_{L^2(\cup T_2)} + \|\gamma R_1 - R_2\|_{L^2(\cup T_2)}.$$

We now consider the rightmost term. Note that

$$\|\gamma R_1 - R_2\|_{L^2(\cup T_2)} \leq \lambda(\cup T_2)|R_1 - R_2| = \frac{\lambda(\cup T_2)}{\lambda(\cup T_2 \cap \cup T_1)}\|\gamma R_1 - R_2\|_{L^2(\cup T_1 \cap \cup T_2)}$$

As mentioned previously, there exists some $\{i(t)\}_{t \in T_1 \cap T_2}$ such that $\nabla v_1 = \gamma(t_i)\nabla v_2$ on $T_1 \cap T_2$. We replace choose γ in the above to γ_i^T. This yields in the above, recalling the expression of v_1 in terms of v_2 that

$$\begin{aligned}\|\gamma R_1 - R_2\|_{L^2(T_1 \cap T_2)} &\leq \|\gamma_{i(t)}^T R_1 - \gamma_{i(t)}^T \nabla v_1 + \nabla v_2 - R_2\|_{L^2(\cup T_1 \cap \cup T_2)} \\ &\leq \sum_{j=1}^{2} \|\nabla v_j - R_j\|_{L^2(\cup T_1 \cap \cup T_2)} \leq \sum_{j=1}^{2} \|\nabla v_j - R_j\|_{L^2(\cup T_j)}.\end{aligned}$$

Combining the above and applying geometric rigidity yields

$$\|V^\omega - \gamma R\|_{L^2(\cup T^\omega)} \leq C\left(\frac{\lambda(T_2)}{\lambda(T_1 \cap T_2)} \max\left(C(\cup T_1), C(\cup T_2)\right)\right) \|\text{dist}(V, \text{SO}(2))\|_{L^2(\cup T^\omega)},$$

where C depends on the number of simply connected regions used. The above can be repeated by induction; as discussed, every T^ω can be broken down into finitely many overlapping simply connected regions as it is locally lattice-like. We deduce that for all locally lattice-like tilings T^ω and their associated symmetric deformation fields, there exists a fixed rotation R^ω, a vector field $\gamma^\omega \in L^2(U, \Gamma)$ and a constant depending on $\cup T^\omega$ such that

$$\|V^\omega - \gamma^\omega R^\omega\|_{L^2(\cup T^\omega)} \leq C(\cup T^\omega) \|\text{dist}(V^\omega, \text{SO}(2))\|_{L^2(\cup T^\omega)}.$$

The proof for general symmetrisable vector fields follows in the same way, with general $\gamma \in L^2(S_j, \Gamma)$ for Lipschitz S_j. On these regions $V \in L^2_{sym}(U)$ is Curl-free and so all the same inequalities hold. $\square$

4.7 The Non-linear Energy of Defects

We now produce some lemmas that allow us to investigate the inclusion of "long range" defect pairs in the statistical mechanical model later, rather than enforce the screening at one fixed length scale. The proofs are largely analytical so they are placed below.

Lemma 4.7.1. *Let $A_{2,1} = B_2 \backslash B_1$ denote an annulus of thickness 1. Suppose $A_1 \subset U$ is a Lipschitz domain such that $U \cup B_1(0)$ is simply connected. Then for all vector fields V that have a non-trivial Frank or Burgers vector around $B_1(0)$, there exists a constant such that*

$$C\|\text{dist} V, \text{SO}(2)\| \geq 1.$$

Moreover, if $V \in L^2(B_n \backslash B_1)$ has the above properties, then for some fixed c_0

$$\|\text{dist}(V, \text{SO}(2))\|^2_{L^2(B_n \backslash B_1)} \geq c_0 \log n.$$

Proof. For any vector field V with a Frank vector the rigidity estimate yields the existence a rotation R such that such that

$$\|\text{dist}(V, \text{SO}(2))\|_{L^2(A_{2,1})} \geq C\|V - \gamma(x)R\|_{L^2(A_{2,1})}$$

where $\gamma \in L^2(U, \Gamma)$. Suppose for a contradiction that there exists a sequence V_n each with Frank vector γ_F such that

$$\min_{R \in \mathrm{SO}(2)} \|(\gamma V)_n(x) - R\|_{L^2(A_{2,1})} \to 0$$

and WLOG we take the rotation above to be the identity. Since the leftmost term is an L^2- bounded sequence, we have V_n weakly converges to a vector field V with

$$\|V - I\|_{L^2(A_{2,1})} \leq \liminf_{n \to \infty} \|V_n - I\|_{L^2(A_{2,1})} = 0.$$

Since γ takes values in a discrete set, it follows $V_n \in \Gamma$ a.e. on U. However, this violates the boundary conditions: it implies that the rotational defect is removable, as vector fields with a non-trivial Frank vector only admit a representation as pointwise rotated gradients in simply connected sets. For a vector field with a non-trivial Burgers vector, set $\gamma = I$ a.e. . The above logic can also be applied: we find that V is globally a gradient field on A_1 contradicting the assumption.

Since the rigidity estimate has a scale-invariant constant, we consider the set of domains $B_2 \backslash B_1$, $B_4 \backslash B_2$,..., and so on up to $B_n \backslash B_{\frac{n}{2}}$. Noting $A_{n,1}$ is the union of these sets, all these domains have the same rigidity constant, and that there are $C \log n$ such domains in this partition of $A_{n,1}$, we find

$$\|\mathrm{dist}(V, \mathrm{SO}(2))\|^2_{L^2(A_{n,1})} \geq \sum_{i=1}^{\log n} \|V - R_i\|^2_{L^2(B(2^i,0) \backslash B(2^{i-1},0))} \geq c_0 \log n.$$

□

In fact, using the knowledge of the behaviour of the rigidity constant above and a trick from Scardia and Zeppieri [2012] allows us to know the behaviour of such a constant in the case of non-trivial Burgers vectors. Suppose that $V \in L^2(A_{n,1}, \mathbb{R}^{2\times 2})$ is such that $\operatorname{curl} V = 0$ with a circulation $b \in N(\mathbb{Z}^2)$ around $\partial B_1(0)$. We have that

$$\|V - R\|_2^2 \geq \int_1^n \frac{1}{2\pi r} \left| \oint_{\partial B_r} (V - R) \cdot t dt \right|^2 dr \geq C|b|^2 \ln n. \tag{4.9}$$

Geometric rigidity on a punctured domain then yields

$$\|\mathrm{dist}(V, \mathrm{SO}(2))\|^2_{L^2(A_{n,1})} \geq C(A_{2,1})|b_x|^2 \ln n. \tag{4.10}$$

Note that if V is defined on $B_n(0)$ with $\operatorname{curl} V \neq 0$ in $B_1(0)$ we have

$$\int_{B_1(0)} |\operatorname{curl} V|^2 \leq C(|\operatorname{curl} V|_\infty)|b_x|^2.$$

This gives a similar result to work in an atomistic model of a screw dislocation, where displacement takes place in the plane above the atoms only. The rigidity estimate yields this linearisation of the energy as opposed to the methods in Hudson and Ortner [2014]. We will use the above estimate after introducing a rigidity estimate for fields with prescribed curl to produce useful statistical estimates for dislocation dipoles As we will have uniform L^∞ results on the extension of a deformation field this gives us a direct comparison between the Burger's vector and the L^2-norm of the curl. Firstly however, we demonstrate a heuristic argument to show the above is not necessarily sharp for disclinations of the kind introduced in Section 3.2.

4.7.1 Rotational Defects in a Large Domain

Let $A_{n,1} = B_n(0)\backslash B_1(0)$. For Curl-free vector fields V with a non-zero Frank vector, then heuristically it should follow that

$$\|\operatorname{dist}(V, \mathrm{SO}(2))\|^2_{L^2(A_n)} = O(n^2),$$

that is, the energy of a rotational defect scales with the system size. To show this, we will assume as in the statistical mechanics section later that $|V| = O(1)$, that is V smoothly varies in A_n. Considering its polar decomposition $V(x) = R(x)U(x)$, intuitively the rotational part should smoothly vary from I to γ_F WLOG. Considering the argument θ of the rotation matrix $R(\theta)$ for a disclination (Figure 3.2) or inspecting the picture shows that in the region ... the rotation is between the two rotations in the symmetry group. There is a "wedge" that scales with system size wherein V takes values that are far from any element of the symmetry group Γ. Recalling the geometric rigidity estimate for symmetrised fields, we see that morally

$$\|\operatorname{dist}(V, \mathrm{SO}(2))\|^2_{L^2(A_{n,n/2})} \geq \|V - \gamma R\|^2_{L^2(A_{n,n/2})} \geq cn^2.$$

where since we consider an annulus of thickness that scales with domain size, this constant is uniform. While we cannot deal with disclinated configurations in full generality, we will use this idea to explain why we believe our results should not be significantly impacted by the presence of disclinations later on. Part of our results are the generalisation of certain inequalities found in Aumann [2015] to not need a rigidity estimate to make conclusions regarding the average energy of the system.

We now introduce a class of rigidity estimates for fields with a prescribed, non-zero curl, as well as provide an estimate on the deformation fields of certain configurations ω that is of particular use to generalise current results found in the literature.

Chapter 5

Rigidity for Vector Fields with Prescribed Curl

5.1 Generalised Rigidity in the Literature

While estimates in the previous chapter will be of some use to us in later results, they depend on both the overall domain U and the location of the hole inside in a way that is not quantified. When there are multiple such holes, randomly distributed around U we cannot produce a uniform rigidity constant. The answer is to develop a rigidity estimate for vector fields with non-zero curl defined on a simply connected domain U, and to consider the behaviour of the rigidity constants involved. For such vector fields, we are interested in quantifying their L^2-distance from a constant rotation in SO(2)- which we deem a measure of the vector field's *orientational order*. As before we wish to consider vector fields whose curl is supported in a relatively small portion of the domain. Before we consider these vector fields we give a brief account of current rigidity estimates found in the literature, then explain why they are not satisfactory for our purposes.

Definition 5.1.1 (r-localised curls)**.** *Suppose U is a simply connected, Lipschitz domain. Let $r > 0$ be given. Let $D \subset U$ denote any finite set in U that satisfies $\operatorname{dist}(x, y) > r + r_m$ for all $x, y \in D$ and some fixed $r_m > 0$. Let $\mathcal{N}(\mathbb{Z}^2) = \mathbb{Z}^2 \cap \overline{B}_1(0)$ denote the unit and zero vectors in the square lattice. We define the set of vector fields with localised curl*

$$\mathcal{L}_r(U) = \left\{ \begin{array}{c} V \in L^2(U),\ \operatorname{curl} V \in L^2(U) : \exists D \text{ with} \operatorname{supp}\operatorname{curl} V \subset \bigcup_{x\in D} B_r(x) \\ b_x := \oint_{\partial B_r(x)} V \cdot dl \in \mathcal{N}(\mathbb{Z}^2) \text{ for all } x \in D \end{array} \right\}$$

In particular we do not enforce that the net Burger's vector associated to V is zero. Moreover, we define the class of $r-$screened vector fields

$$S_r(U) = \{V \in L^2(U), \operatorname{curl} V \in L^2(U), \exists D : \oint_{\partial B_r(x)} V \cdot dl = 0 \, \textit{for all} \, x \in D\}$$

We will call the set D the *defect set* of V. While ultimately we will consider a certain subset of $\mathcal{L}_r(U)$, it is possible to prove a rigidity estimate for a larger class of vector fields that is quantitatively better than ones stated in the literature currently, as well as one that can be applied to a family of different domains. Ultimately we wish to consider a "large" crystal whose defects are always approximately the same size, coming from the properties of the lattice $\mathbb{Z}^2$ as discussed previously. We will now discuss the problem with rigidity estimates and their generalisation to translational defects, that is we work in the framework of Definition 5.3.1.

5.1.1 The Problem

Let U_1 be some fixed, Lipschitz domain. We consider, for fixed r, the spaces $\mathcal{L}_r(nU_1)$ and $S_r(nU_1)$ for some fixed U_1 and $n \geq 1$. The geometric rigidity theorem for incompatible fields,obtained in Aumann [2015] for general p and Müller et al. [2014] for $p = 2$ yields for each $V \in L^2(U_n)$ the existence of a rotation such that

$$\|V - R\|_{L^2(U_n)} \leq C(U_1)\|\operatorname{dist}(V, SO(2))\|_{L^2(U_n)} + C_2(n,p)\|\operatorname{curl} V\|_{L^p(U_n)}.$$

For higher dimensional analogues of this see Lauteri and Luckhaus [2017]. This gives us a family of inequalities, indexed by n for general fields $V \in L^2(U_n)$.While the first constant on the right hand side is the same for all U_n, it is the behaviour of the second constant that must be considered to use this estimate for a family of problems. In our application it is advantageous to measure curl in the L^2-norm as we will show shortly. Moreover, we require the estimate to be *uniform* in n in order to estimate the left hand side accurately enough for our purposes. However, the existing estimates (Aumann [2015],Müller et al. [2014]) yield that for each $V \in L^2(U_n, \mathbb{R}^{2\times 2})$

$$\|V - R\|_{L^2(U_n)} \leq C_1(U_1)(\|\operatorname{dist}(V, SO(2))\| + n\|\operatorname{curl} V\|_{L^2(U_n)}). \tag{5.1}$$

Consider a vector field $V \in L^2_{loc}(\mathbb{R}^2, \mathbb{R}^{2\times 2})$ which is identically equal to a rotation outside of a small region $B \subset U_1$ where V possesses a curl. Clearly the rigidity estimate must provide this R such that $\|V_n - R\|_2 = O(1)$ for all large enough

$n \in \mathbb{N}$. However, the rigidity estimate yields that

$$O(1) = \|V - R\|_{L^2(U_n)} \lesssim O(n),$$

and we lose control over the left hand side if we use the rigidity estimate as an upper bound. The alternative rigidity estimate from Aumann [2015] in which we measure curl with $p = 1$ removes the n-dependence, yielding

$$\|V - R\|_{L^2(U_n)} \leq C(U_1)\|\mathrm{dist}(V, SO(2))\|_{L^2(U_n)} + C_2\| \operatorname{curl} V\|_{L^1(U_n)}.$$

However, now suppose the vector field $V \in L^2_{loc}(\mathbb{R}^2, \mathbb{R}^{2\times 2})$ possesses many defects, say lying in small balls around points in the lattice $\mathbb{Z}^2$, then $\lambda_2(\operatorname{supp} \operatorname{curl} V) = C\lambda_2(U_n)$. Let these points be denoted by D. Again assuming it co-incides with a rotation outside this region[1], we find the estimate is sub-optimal:

$$O(\#D^{1/2}) = \|V - R\|_{L^2(U_n)} \lesssim O(\#D^{1/2}) + O(\#D).$$

Since in principle we expect a finite density of defects in a statistical model of a crystal at finite temperature (see for instance the energy-entropy arguments in Chapter 13 of Kosevich [2006]), it is for this reason that we derive a different estimate. In particular, we wish to find conditions on vector fields for when we are able to control the order of vector fields uniformly for $n \in \mathbb{N}$ in L^2 while admitting a finite density of defects. As a short introduction to this chapter, we demonstrate the following and similar results. As these estimates are usually used in plasticity models (Scardia and Zeppieri [2012], Müller et al. [2014]) it is of no great surprise that it is difficult to use them directly for equilibrium mechanics. Usually results are shown in a norm or energy scaling that does not detect 'dipoles' as it is the unbound dislocations and their higher strain fields that are of interest.

Theorem 5.1.2 (Rigidity for Screened Vector Fields)**.** *For every $V \in S_r(U_n)$ there exists some fixed rotation $R \in \mathrm{SO}(2)$ such that*

$$\|V - R\|_{L^2(U_n)} \leq C(U_1, r)(\|\mathrm{dist}(V, \mathrm{SO}(2)))\|_{L^2(U_n)} + \| \operatorname{curl} V\|_{L^2(U_n)}).$$

Importantly for our purposes, the constant in the estimate above does not depend on system size n. That is, we place vector fields with "small" regions of curl in a large domain, and find the estimate is insensitive to how large the domain

[1] A means to construct such a vector field rigorously using a solution to Poisson's equation with any zero-mean source f contained in a small support is given in the next section.

is or the other properties of $\operatorname{supp}\operatorname{curl} V$ (besides the screening and a spacing condition). Note that r is always the same value for any domain U in this notation. The benefit of such an estimate is easily seen. Returning to the heuristic calculations above, again take the vector field $V \in L^2_{loc}(\mathbb{R}^2, \mathbb{R}^{2\times 2})$ possessing defects with $\lambda_2(\operatorname{supp}\operatorname{curl} V) = C\lambda_2(U_n)$. Rigidity for screened vector fields yields regardless of the choice of n that

$$O(\sqrt{\#D}) = \|V - R\|_{L^2(U_n)} \lesssim O(\sqrt{\#D}).$$

5.2 Rigidity, Scaling, and Unscreened Defects

5.2.1 Rigidity Estimates and Scaling

We now give a brief account of why the discrepancy between the estimate 5.1.2 and the one for general vector fields arises. Let $V_1 \in S_r(U_1)$ and let $y \in U_n$. Define the function $V : U_n \to \mathbb{R}^{2\times 2}$ by $V(y) = V_1(n^{-1}y)$. Applying this procedure to every $V \in S_r(U_1)$ yields a space $S'(U_n)$. It is clear that

$$S'(U_n) \subset \{V : \operatorname{supp}\operatorname{curl} V \subset \bigcup_{x_i \in D_1} B_{nr}(nx_i), \quad B_i \text{ disjoint.}\}.$$

We see that since $V \notin S_r(U_n)$ there is no contradiction with the estimate in Equation (5.1). Rather, rigidity for vector fields in general is not sharp for screened or admissible vector fields (introduced later, based on the admissible configurations in Section 2.12). We now demonstrate that how the requirement $V \in \mathcal{L}_r(U)$ delivers a different bound for the quantity $\|V - R\|_{L^2}$, following the idea of Müller et al. [2014].

5.2.2 Rigidity for A Single Defect

In a similar fashion to the rigidity estimate for punctured domains, we now produce a rigidity estimate for a single defect occupying a small ball. Suppose WLOG that $0 \in U_1$. For concreteness let $f \in L^2(U_1, \mathbb{R}^2)$ be such that $D := \operatorname{supp} f = B_r(0)$. This will play the role of our defect. We wish to study all fields that we specify to possess this and only this defect:

$$A(f) = \bigcup_{n=1}^{\infty} \{V \in \mathcal{L}_r(U_n) : \operatorname{curl} V = f.\}$$

Then for every $V \in A(f)$ we will show that for the appropriate n the inequality

$$\|V - R\|_{L^2(U_n)} \leq C(U_1)\|\mathrm{dist}(V, \mathrm{SO}(2))\|_{L^2(U_n)} + Cr(\log(r^{-1}\mathrm{diam}(U)))\|f\|_{L^2(U_n)}$$

holds. To do this, we will outline the proof of the rigidity estimate found in Müller et al. [2014], with some modifications. Consider Poisson's equation

$$\begin{cases} -\Delta u = f \text{ in the plane,} \\ u \in H^2_{loc}(\mathbb{R}^2; \mathbb{R}^2). \end{cases}$$

Given the existence of such a u, we take the matrix and the vector field

$$J = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}, \quad W = \nabla u J.$$

Then $W = \nabla u J$ is such that $\operatorname{curl} W = \operatorname{curl} V$. Since by assumption nU_1 is simply connected, for any $V \in A(f)$ there exists a function $\varphi \in H^1(U_n, \mathbb{R}^2)$ such that the difference $W\chi(U_n) - V = \nabla\varphi$ on U_n. Applying the rigidity estimate used in the introduction, Equation (4.1), for gradients (c.f. Friesecke et al. [2002]) and rearranging yields the existence of a rotation R such that

$$\|V - R\|_{L^2(U_n)} \leq C_{RIG}(U_1)\|\mathrm{dist}(V, \mathrm{SO}(2))\|_{L^2(U_n)} + 2C_{RIG}(U_1)\|W\|_{L^2(U_n)},$$

making use of the fact that the constant for this rigidity estimate is scale invariant. The function we will use that satisfies the above will be the fundamental solution (c.f. 7.1)

$$u(x) = -\frac{1}{2\pi}\int_{B_r(0)} f(y) \ln|x - y| \,\mathrm{d}y.$$

The gradient of the potential is square integrable whenever $x - y \in B_r(0)$. On the one hand, by Young's inequality

$$\|\nabla u\|_{L^2(U_n)} \leq \|\nabla\Phi\|_{L^1(U_n)}\|f\|_{L^2(U_n)} \approx n\|f\|_2,$$

which is the result given by a scaling argument. On the other hand, we have

$$\|\nabla u\|_{L^2(U_n \setminus B_r(0))} \leq \|\nabla\Phi\|_2\|f\|_1 \approx C\ln(r^{-1}n)\|f\|_1.$$

We would also like to measure f in L^2 while retaining the logarithmic factor. To do this we split the field up as follows:

$$W = W\chi(B_{2r}(0)) + W\chi(U\backslash B_{2r}(0)).$$

Recall W is defined through the convolution

$$W\chi(B_{2r}(0)) = \int f(y)\Phi(x-y)\chi[B_2r(0)](x)\,\mathrm{d}y.$$

For $x \in B_{2r}(0)$, the rightmost term is not square integrable but is integrable. We therefore apply Young's inequality in this ball to yield

$$\|W\|_{L^2(B_{2r})} \leq Cr\|f\|_2.$$

Outside of this ball, both functions are square integrable and we find

$$|\partial_i u_j(x)|^2 \leq \|f\|^2_{L^2(B_r(0))}\|\Phi(x-y)\|^2_{L^2(B_r(0);y)} \leq Cr^2\|f\|_{L^2}|\Phi(x)|^2.$$

Integrating both sides over $U_n\backslash B_r(0)$, taking square roots and using the triangle inequality yields

$$\|W\|_{L^2(U)} \leq r\|f\|_2(C_1 + C_2(\ln r^{-1}n)).$$

We can see from this that we recover the scaling argument if we look at curl supported in a ball of radius proportional to n. However for the special case of "point" defects in a large domain we get a better estimate. Once again this estimate is not sharp for defects. The norm of the vector field W depends on the circulation of V, or rather the integral of f. In the above we have a single, *unscreened* defect, $\int f = \neq 0$. For the class of fields

$$A(f_0) = \cup_n\{V \in \mathcal{L}_r(U_n) : \operatorname{curl} V = f_0, \mathrm{supp} f_0 \subset B_r(0), \int f_0 = 0\},$$

it is possible to show that $\|W\|^2_{L^2(\mathbb{R}^2)} \leq Cr^2$ (Lemma 7.0.3). Combining the above estimates gives

$$\|V - R\|_{L^2(U_n)} \leq C(U_1)(\|\mathrm{dist}(V, \mathrm{SO}(2))\|_{L^2(U_n)} + r\|\operatorname{curl} V\|_{L^2(U_n)}).$$

We now generalise this framework to the case where V possesses many defects of different kinds. In particular, we produce a useful estimate for when V is the local deformation of an admissible configuration, as well as another analytical estimates.

5.3 Vector Fields, Defect Sets and Partitions

In this section we develop some notation to characterise the defect set of fields with localised curl. Recall the definition

Definition 5.3.1 (r-localised curls). *Suppose U is a simply connected, Lipschitz domain. Let $r > 0$ be given. Let $D \subset U$ denote any finite set in U that satisfies* $\operatorname{dist}(x, y) > r + r_m$ *for all $x, y \in D$ and some fixed $r_m > 0$. Let $\mathcal{N}(\mathbb{Z}^2) = \mathbb{Z}^2 \cap \overline{B}_1(0)$ denote the unit and zero vectors in the square lattice. We define the set of vector fields with localised curl*

$$\mathcal{L}_r(U) = \left\{ \begin{array}{c} V \in L^2(U),\ \operatorname{curl} V \in L^2(U) : \exists D \text{ with} \operatorname{supp}\operatorname{curl} V \subset \bigcup_{x\in D} B_r(x) \\ b_x := \oint_{\partial B_r(x)} V \cdot dl \in \mathcal{N}(\mathbb{Z}^2) \text{ for all } x \in D \end{array} \right\}$$

Definition 5.3.2 (Defect Set). *Let $V \in L_r(U)$. We call the finite set D above the defect set.*

Some further assumptions on the structure of the curl allow us to prove a quantitatively better estimate for an appropriate subclass of r-localised fields. We now develop some notation and definitions as preparation for stating Theorem 5.6.2, and point out where generalisations can be made if more complicated notation is developed.

5.3.1 Defects and Defect Pairs

In addition to the case of screened vector fields, we are interested in vector fields whose curls screen each other out, but not over a fixed length scale. Motivated by various results in both the analysis and statistical mechanics of dislocations, we will define a class of vector fields for which an estimate that respects the structure of their curl can be proved. First we develop some notation.

Definition 5.3.3 (Burgers vector of a defect). *Let $V \in \mathcal{L}_r(U)$. Let $x \in D$. We define the vector*

$$b_x = \int_{B_r(x)} V \cdot dl \in \mathcal{N}(\mathbb{Z}^2).$$

Should we label the points in D by $x_i, i \in N$ we instead refer to the above quantity as b_i.

Definition 5.3.4 (Defect Pair)**.** *Let U be a simply connected, Lipschitz domain. We say two defects $x_1, x_2 \in D$ form a pair if*

$$\int_{B_r(x_1)} \operatorname{curl} V = -\int_{B_r(x_2)} \operatorname{curl} V, \quad \int_{B_r(x_i)} |\operatorname{curl} V| \neq 0.$$

5.3.2 Partitioning the Defect Set

The discussion in Section 5.2.2 highlights the need to treat different kinds of defects separately. Defects that screen each other contribute smaller terms to the right hand side of the inequality. To this end we look for a partition of the defect set D into sets D_0, D_p and D_s. In particular, the partition will be such that

$$D_0 = \{x_i : b_i = 0\},$$

$$D_p = \{(x, y) : (x, y) \text{ is a paired defect, } x, y \text{ belong to exactly one pair } \forall x, y\},$$

$$D_s = D \backslash (D_p \cup D_0)$$

and the cardinality of D_p is maximised. While it is clear such a partition always exists, it is of course not unique. The idea will be to pair defects in a judicious way- we wish for the set D_s to be as "isolated" as possible. In this framework it represents unpaired dislocations that will contribute a large term to the right hand side of the rigidity estimate. If defects are close to each other and can be paired, they should be placed in D_p. As long as we collect all defects with no net Burgers vector into D_0, it is unique. To find choices of D_p, D_s such that the points in D_s are 'isolated', we follow a similar idea to Hudson and Ortner [2014]. We minimise the total difference between points in D_p:

$$D_p^* = \operatorname{argmin}_{D_p} \sum_{(x,y) \in D_p} |x - y|.$$

This means that if we have a "cluster" of defects so that V has no net circulation around it, and a few far away isolated defects possessing the same value b, the optimal sets will be such that D_p is this cluster and D_s is the far away defects, seen in Figure 5.1. Clearly at last one best choice of D_s, D_p exists as there are finitely many choices of D_p, but may still be non unique. As a matter of preference we choose any D_p such that all pairs have disjoint neighbourhoods. If that is still not unique, we pick one by a fixed rule (for instance, uniformly at random). This can occur where there the b_i sum to zero, but they are arranged in a square where each corner is alternately b^1 and $-b^1$, say. We now define what is meant by the

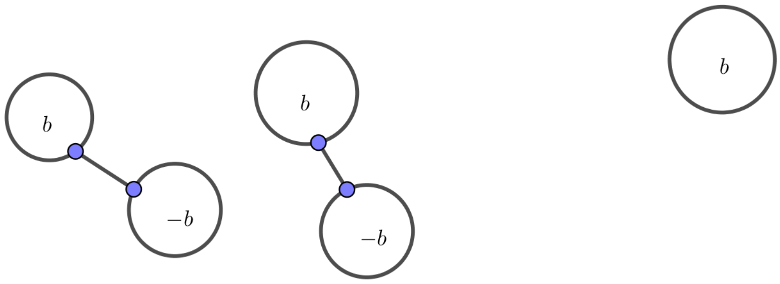


Figure 5.1: Choosing a cluster minimises the total "length" of D_p. There is no reason to expect uniqueness of these sets.

neighbourhood of a defect or a defect pair. These sets are needed to establish the rigidity estimate in Theorem 5.6.2.

5.3.3 Regular Neighbourhoods and Admissible Vector Fields

As we work with vector fields with curls in $L^2(U)$ we must prescribe continuum domains to defects or defect pairs. As it is important for the rigidity estimates later, we will ensure they are disjoint. Ultimately we will consider a subset of $\mathcal{L}_r(U)$ whose neighbourhoods of defects satisfy an appropriate regularity condition. To start with we make two definitions.

Definition 5.3.5 (Regular Neighbourhoods)**.** *Let $x, y \subset \mathbb{R}^2$ and let $r > 0$ be given. Let $N(x,y)$ be a simply connected, C^1-domain containing x and y with* $\operatorname{dist}(x, \partial N(x,y)) = 2r, \operatorname{dist}(y, \partial N(x,y)) = 2r$. *Let*

$$N_r = \{a \in N(x,y) : \operatorname{dist}(a, \partial N(x,y)) \geq r\}.$$

We say $N(x,y)$ is an r-regular neighbourhood of (x,y) if $\operatorname{dist}(a, \partial N(x,y)) \leq 2r$ *for all $a \in N(x,y)$ and there exists a function $\eta \in C_c^1(U)$ with $\eta = 1$ on N_r, $\eta = 0$ on $N(x,y)^c$ and $|\nabla \eta(a)| \to 0$ as $a \to \partial N_r$ and $a \to \partial N$.*

Definition 5.3.6. *To defects consisting of a single point we associate the neighbourhood $N(x) = B_r(x)$.*

Definition 5.3.7. *For vector fields with a single defect pair we associate the line neighbourhood*

$$N_r(x_1, x_2) = \{y : \operatorname{dist}(y, \ell) \leq r\} \text{ with } \ell = \{x : x = x_1 + t(x_2 - x_1),\ t \in [0,1]\}$$

that is, all points that lie a distance of at most r from the line connecting x_1 *and* x_2 *for some pair* (x_1, x_2)*.*

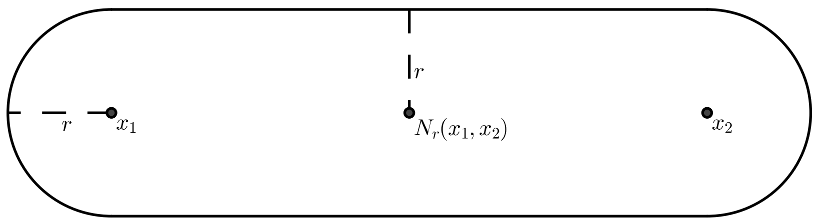


Figure 5.2: A diagram of $N_r(x_1, x_2)$ for some $x_1, x_2 \in \mathbb{R}^2$. $\partial N_r(x_1, x_2)$ is shown by a solid line.

As we will see both of these neighbourhoods are $r/2$-regular. We now define the admissible vector fields and note that all admissible configurations produce an admissible vector field V^ω (up to multiplication by a global rotation and some $\gamma \in L^2(\cup T, \Gamma)$).

Definition 5.3.8 (Admissible Vector Fields)**.** *Let* $r, r_{min} > 0$ *be given and let* U *be a simply connected, Lipschitz domain. We let* $A_{r,\alpha}(U) \subset \mathcal{L}_r(U) \oplus S_\alpha(U)$ *be the set of vector fields such that for all* $V \in A_{r,\alpha}(U)$ *there exists a disjoint family of regular neighbourhoods* $\{N(p)\}$ *for* $p \in D_p$*, and* $\operatorname{dist}(N(p_1), N(p_2)) > r_m$ *for all distinct* p_i*.*

The reason for the construction of neighbourhoods is to define an appropriate cut-off function on a neighbourhood inside of which a vector field possesses 0 net Burgers vector. This cut-off function must have a $W^{1,\infty}-$norm that is uniformly bounded with respect to a parameter r_{min}. We now give an example of a vector field in $A_{r,\alpha}(U)$ despite the fact a line neighbourhood cannot be used.

5.3.4 Example of a Field in $A_{r,\alpha}(U)$

An example where the neighbourhoods of paired defects is not disjoint if line neighbourhoods are used is presented in the image below:

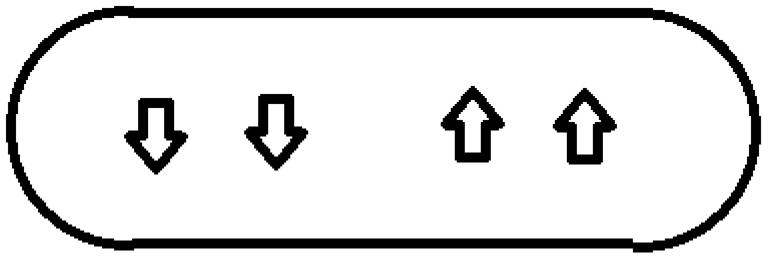


Figure 5.3: An example of a defect set that would yield a vector field not in $\tilde{A}_r$

It is intuitively clear that this arrangement should pose no real problems besides notational ones. We can either absorb the two “sides” into balls of double radius and Burgers vector then pair them, or produce a neighbourhood built out of balls, linear sections and annuli. For the latter option, this defect can be dealt with in our framework by using curved neighbourhoods as drawn below. This results in disjoint neighbourhoods on which a cut-off function that behaves appropriately can be defined. It will be seen later that the result in Theorem 5.6.2 would still hold with the same bound for any appropriate choice of disjoint, regular neighbourhoods.

5.4 Admissible Configurations and Vector Fields

Theorem 5.4.1. *Let $\omega \in \Omega_n$ be an admissible configuration in the sense of Section 2.12. For every ω there exists a local deformation $V^\omega \in A_{r,\alpha}(U_n)$.*

Proof. Due to the consistent ordering condition on admissible fields and its regularity, we can pick some set of values V^ω to receive a curl-free vector field on $\cup T^\omega$. Clearly the defect set $D^\omega = U_n \backslash T^\omega$ has properties that match that of $\operatorname{supp} \operatorname{curl} V$ for $V \in A_{r,\alpha}(U_n)$ for appropriate parameter choices of the screened and paired defect sizes. The only question is whether appropriate neighbourhoods of defects can be defined. As in the definition of the defect sets for vector fields, we identify D^ω with the finite sets D_0^ω and D_p^ω with $D_s^\omega = \varnothing$. We take D_0^ω to be the centres of the balls of the screened part of the defect set and D_p^ω to be any pairing of the defects. We recall the relevant properties of the admissible configurations: there exists a finite sets I_1, I_2 and numbers $r_m, \alpha_0, \alpha_1, \alpha_2$ such that

- D^ω can be covered such that

$$D^\omega \subset \bigcup_{x \in I_0} B_{\alpha_0}(x) \cup \bigcup_{x \in I_p} B_{\alpha_p}(x)$$

- D^ω has a disjoint partition into sets D_0^ω and D_p^ω with

$$\text{dist}(x, y) > \alpha_0 + r_m \text{ for all } x, y \in I \cap D_0^\omega$$

and that $D_p^\omega = \{(d_1, d_2), ..., (d_{2K(\omega)-1}, d_{2K})\}$ for some $K(\omega) \in \mathbb{N}$ such that $d_i \subset B_{\alpha_p}(x)$ for all i, and

for each pair (d_k, d_{k+1}) $\exists \rho(\omega) : C\rho(\omega) \geq \text{dist}(d_k, d_{k+1}) > \rho(\omega) > 2(\alpha_p + r_m) \forall i, j$

Due to the minimum mutual condition on D_p^ω, there exists a pairing D_p^* such that $\text{dist}(x, y) > \rho > 2r_m$ for all pairs $(x, y) \in D_p^\omega$. Along the line connecting these two defects, there can be no other elements in D_p^ω, only defects in D_0^ω (otherwise there would exist y' with $\text{dist}(x, y') < \rho$). It follows that using the linear neighbourhoods in Definition 5.3.7 result in disjoint, regular neighbourhoods for D_p^ω. Since each defect in D_p^ω belongs to exactly one pair, we have our disjoint regular neighbourhoods. As we will see, it does not matter that these are not disjoint with the neighbourhoods of elements in D_0^ω. $\square$

5.5 $A_{r,\alpha}(U) \neq \mathcal{L}_r(U) \oplus S_\alpha(U)$

For completeness we demonstrate that not all localised vector fields are admissible. Let " + " denote $(1, 0)$ and " − " denote $(-1, 0)$. Consider a vector field

$$\oint_{\partial B_r(x)} V = \pm, \ x \in D,$$

where V has a curl has the form presented in Figure 5.4. It is such that $D_0 = D_s = \varnothing$.

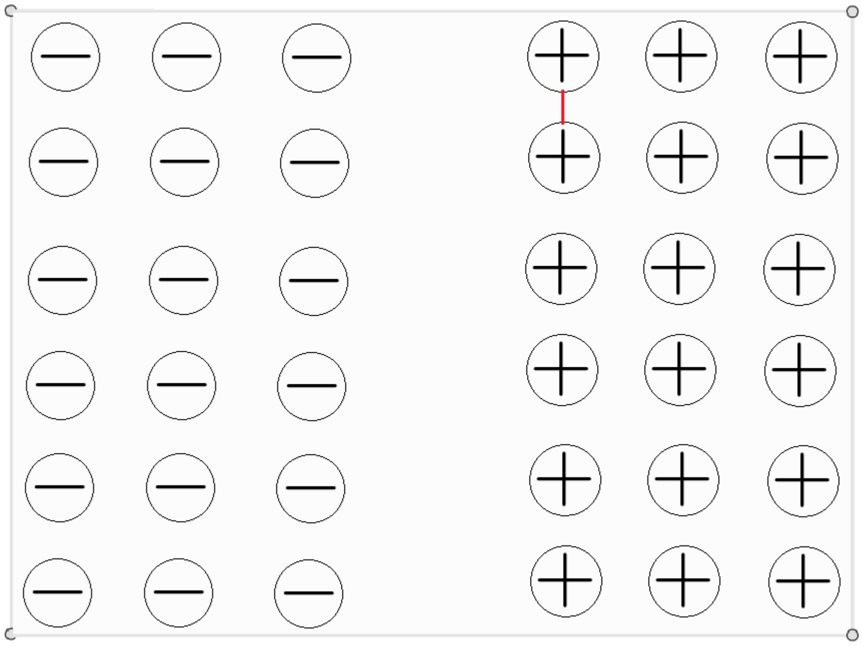


Figure 5.4: A vector field whose curl is localised but not admissible

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Define the flux $F(\ell)$ of a line ℓ by the number of neighbourhoods that cross through it. For the edge highlighted in Figure 5.4 it is clear that we must choose $F(\ell) \geq Cw$ where w is the width of the shaded rectangle. If this were not true another line on the edge of the shaded region must have a strictly greater flux. For a fixed core size r and a large enough box, we lose control of the neighbourhood width and must take neighbourhoods $N_r(x, y)$, $r \to 0$ if they are to be disjoint. This causes the $W^{1,\infty}$-norm of any cut-off function defined on these neighbourhoods to blow up as its gradient is bounded by a negative power of r. As we will see this would lose control of the left hand side of any rigidity estimate produced by the methods in this thesis.

5.6 Rigidity For Admissible Vector Fields

We now give the full statement of the rigidity theorem for screened and admissible vector fields. A discussion of the results follows, and the proofs of underlying L^2-estimates needed are found in Chapter 7. For screened vector fields we use the screening parameter α rather than r. This is to emphasise the fact that, in admissible configurations, α need not be the size of an individual defect of radius r. We need only that there exists some fixed α that screens clusters of defects and the minimum spacing conditions.

Theorem 5.6.1 (Geometric Rigidity for α-Screened Fields)**.** *Let U be a simply connected domain with a Lipschitz boundary and suppose that $V \in S_\alpha(U)$ with some minimum spacing r_m. For any such V there exists a rotation $R \in \mathrm{SO}(2)$ such that*

$$\|V - R\|_{L^2(U)} \leq C(U)(\|\mathrm{dist}(V, \mathrm{SO}(2)))\|_{L^2(U)} + \alpha C(r_m)\|f\|_{L^2(U)}),$$

and $C(U) = C(\eta U)$ for all $\eta > 0$ and all $V \in S_r(\eta U; r_m)$.

Theorem 5.6.2 (Geometric Rigidity for Admissible Fields)**.** *Let U be a simply connected domain with a Lipschitz boundary and suppose $V \in A_{r,\alpha}(U)$ as in Section 5.3.1. Then for each such V there exists a constant rotation $R \in \mathrm{SO}(2)$ satisfying*

$$\|V - R\|_{L^2(U)} \leq C_1(U)(\|\mathrm{dist}(V, SO(2))\|_{L^2(U)} + rE(\mathrm{curl}\, V)),$$

where for $f \in L^2(\mathbb{R}^2)$ with $\mathrm{supp} f \subset \cup_{x \in D} N(x)$, $\int_{N(x)} f = b_x$,

$$E(f)^2 = r^{-1}\alpha\|f\|^2_{N_\alpha(D_0)} + \sum_{(x,y)\in D_p} \log(|x-y|)\|f\|^2_{N(x,y)} + (|D_s| \log\left(r^{-1}\mathrm{diam}(U)\right))\|f\|^2_{N(D_s)}.$$

Here, all norms are the L^2-norm, $N(D) = \cup_{x\in D} N(x)$, and the sets D_0, D_p, D_s are defined in Section 5.3.1. In the above, $C_1(\eta U) = C_1(U)$ for all $\eta > 0$ and for $V \in A_{r,\alpha}(\eta U)$.

N.B: Should $r < \mathrm{diam}(U) < 1$ or $\mathrm{dist}(x_1, x_2) < 1$ the relevant logarithmic terms must be replaced by 1.

Corollary 5.6.3 (Geometric Rigidity for Vector Fields II)**.** *Let U be a simply connected, Lipschitz domain. For every $V \in L^2_{\mathrm{curl}}(U)$ there exists a constant rotation R such that*

$$\|V - R\|_{L^2(U_n)} \leq C(U)(\|\mathrm{dist}(V, \mathrm{SO}(2))\|_{L^2(U_n)} + \mathrm{diam}(U)\|\,\mathrm{curl}\, V\|_{L^2(U_n)}),$$

where $C(U) = C(\eta U)$ for all $\eta > 0$.

5.7 Proof of Rigidity Theorems

Proof of Theorem 5.6.1. After proving the result for screened vector fields, it will be straightforward to prove the result for paired ones. To this end, suppose $V \in S_\alpha(U)$

is a screened vector field. We claim there exists a vector field W supported on $\cup_i B_{\alpha+\frac{1}{2}r_m}(x_i)$ such that $\operatorname{curl} W = \operatorname{curl} V := f$ and

$$\|W\|_{L^2(\mathbb{R}^2)} \leq C\|f\|_{L^2(U)}.$$

Since $\operatorname{curl}(V-W) = 0$ on U, We can apply Theorem 4.2.1 to the difference to yield the existence of a rotation $R \in SO(2)$ such that

$$\begin{aligned}\|V-R\|_{L^2(U)} &\leq C\|\operatorname{dist}(V-W, \mathrm{SO}(2))\|_{L^2(U)} + C\|W\|_{L^2(U)}\\ &\leq C(\|\operatorname{dist}(V, \mathrm{SO}(2)))\|_{L^2(U)} + \alpha\|f\|_{L^2(U)}),\end{aligned}$$

where C is the same for all $V \in A_{r,\alpha}(\eta U)$ for any $\eta > 0$. □

Proof of Claim. As before, let $f := \operatorname{curl} V$. By assumption, $\operatorname{supp} f$ is covered by disjoint balls of radius α separated by a parameter r_m. Consider the set of Poisson's equations for $x_i \in D$

$$\begin{cases} -\Delta u^i = f\chi(B_\alpha(x_i)) := f^i \\ u \in H^2_{loc}(U, \mathbb{R}^2), \ \int f^i = 0. \end{cases}$$

We consider the vector field $\nabla u^i J\chi(B_{\alpha+r_m})$where J is the rotation matrix introduced in section 5.2.2. Note that in B_α we cannot write the vector field ∇uJ as a gradient. However in $B_{\alpha+r_m}\backslash B_\alpha$, ∇uJ is path independent: it follows that there exists a potential ϕ^i such that $\nabla u^i J = \nabla\phi^i$. Define the vector fields

$$W^i = \begin{cases} \nabla u^i J, \text{ on } \overline{B_\alpha}, \\ \nabla(\eta\phi^i), \text{ on } B_{\alpha+r_m}\backslash B_\alpha, \\ 0, \text{ otherwise.} \end{cases}$$

here η is a cut-off function supported on $B_{\alpha+\frac{1}{2}r_m}$ such that $\eta = 1$ on B_α, $\eta = 0$ on $\partial B_{\alpha+\frac{1}{2}r_m}$ and

$$\lim_{x\to\partial B_\alpha} \nabla\eta(x) = 0 = \lim_{x\to\partial B(x_i,\alpha+\frac{1}{2}r_m)} \nabla\eta(x).$$

For instance, for the ball $B(0,2)$ this can be achieved by the radial cut-off function

$$\eta(r) = \begin{cases} 1, \ r \leq 1 \\ \exp\frac{-1}{1-(r-1)^2}, \ 1 < r < 2 \\ 0, \text{ otherwise.} \end{cases}$$

and readily generalised by taking $\tilde{\eta}(x) = \eta(c|x - x_i|)$, with $c = \frac{1}{2}(\alpha + \frac{1}{2}r_m)$. We assume then that we are given such a cut-off function with $\nabla\eta = 0$ on $B_\alpha \cup \partial B_{\alpha+\frac{1}{2}r_m}$, and η is continuously differentiable. We have

$$\nabla(\eta\phi^i) = \eta\nabla\phi^i + \begin{pmatrix} \phi^i_1\partial_1\eta & \phi^i_1\partial_2\eta \\ \phi^i_2\partial_1\eta & \phi^i_2\partial_2\eta \end{pmatrix} \tag{5.2}$$

Since u^i and entries in Du^i are bounded on $B_{\alpha+r_m}\backslash B_\alpha$ and thanks to the representation above for ϕ^i, the ∞-Poincaré inequality yields that $|\phi^i|_\infty \le C|\nabla u^i|_\infty < \infty$ in $B_{\alpha+\frac{1}{2}r_m}\backslash B_\alpha$.

Since ϕ is bounded, the rightmost term in equation (5.2) becomes 0 on the boundary of $B_{\alpha+\frac{1}{2}r_m}\backslash B_\alpha$. It follows that the W^i are continuous vector fields and piecewise H^1, whence $W \in H^1(U)$. As claimed, $\mathrm{supp} W_i = B_{\alpha+\frac{1}{2}r_m}(x_i)$. As the weak derivatives of W exist and co-incide with the piecewise definition a.e., by construction then $\operatorname{curl} W^i = f^i$: outside of B_α the W^i are gradients, and the curl of a gradient is equal to 0. It follows that for the vector field $W = \sum_i W^i$, $\operatorname{curl} W = f = \operatorname{curl} V$.

By assumption the W^i have disjoint support, whence

$$\|W\|^2_{L^2(U)} = \sum_i \|W^i\|^2_{L^2(U)} \le \alpha\|\eta\|_{W^{1,\infty}} \sum_i \|f^i\|^2_{L^2(U)} \le C(r_m)\alpha\|f\|^2_{L^2(U)}.$$

The bound on $\|W^i\|_{L^2(U_n)}$ follows from Lemma 7.0.4. This proves the claim. $\square$

Proof of Theorem 5.6.2. Assume WLOG that V only has two defects total. Consider Poisson's equation:

$$\begin{cases} -\Delta u = f\chi(B_1) + f\chi(B_2), \\ u \in H^2_{loc}(U, \mathbb{R}^2), \quad \int f = 0. \end{cases}$$

We take the pair $\pi = (x_1, x_2)$ and define $\nabla uJ\chi(N_{2r+r_m}(x,y))$, where $N(x,y)$ is the neighbourhood constructed in subsection 5.3.1, with parameter $2r + r_m$. As before, note that in $N_r(x,y)$ we cannot write the vector field $\nabla uJ\chi(N_{2r+r_m}(x,y))$ as a gradient. However in $N_{2r+r_m}(x,y)\backslash N_r(x,y)$, ∇uJ is path independent: There exists a potential ϕ such that $\nabla u J = \nabla \phi$. Define the vector field

$$W^p = \begin{cases} \nabla u J, \text{ on } \overline{N_r}, \\ \nabla(\eta\varphi), \text{ on } N_{2r+\frac{1}{2}r_m}(x,y) \backslash N_r(x,y), \\ 0, \text{ otherwise.} \end{cases}$$

where η is a cut-off function supported on $N_{2r+\frac{1}{2}r_m}(x,y)$ with the same decay properties as in the case for screened defects. For completeness, such a function can be constructed as below: Assume that $x = (0,0)$ and $y = (0,1)$ for simplicity. Define

$$\eta(x_1,x_2) = \begin{cases} 1, \ (x_1,x_2) \in N_1(x,y) \\ \exp\{\frac{-1}{1-|x_1|^2}\}, 1 \leq |x_1| \leq 2, \ \ 0 \leq x_2 \leq 1 \\ \exp\left\{\frac{-1}{1-\operatorname{dist}^2((x_1,x_2),\partial N_1(x,y))}\right\}, (x_1,x_2) \in N_2(x,y)\backslash([-1,1]\times[0,1]) \cap \{(x_1,x_2) : x_2 > 0\} \\ \exp\left\{\frac{-1}{1-\operatorname{dist}^2((x_1,x_2),\partial N_1(x,y))}\right\}, (x_1,x_2) \in N_2(x,y)\backslash([-1,1]\times[0,1]) \cap \{(x_1,x_2) : x_2 < 0\} \end{cases}$$

Choosing appropriate co-ordinates we see η retains the correct properties. Scaling, translation, and rotation yields the result for general line neighbourhoods. From the same logic as in the previous proof, we receive a vector field W^p with $\operatorname{curl} W^p = f$. The bound $\|W_p\|_{L^2(U_n)}$ follows from Lemma 7.0.4, yielding that

$$\|W\|^2_{L^2(N_{2r})} \leq \|W\|^2_{L^2(\mathbb{R}^2)} \leq C(r_m) r \log(|x(p_1) - x(p_2)|)\|f\|^2_U.$$

Now suppose that $V \in A_{r,\alpha}(U)$ is such that $D_s = \varnothing$. Recall that the support of its curl is broken down using a partition of pairs and singletons. We assume as in the statement of the theorem that neighbourhoods of defects pairs are disjoint, and that a regular enough cut-off function exists for each neighbourhood. We then construct the set of fields $W^p : p \in D_0, D_p$ as in the previous two proofs for defects in D_0, D_p respectively. Then $\operatorname{curl}(V - \sum_p W^p) = 0$ as before, and by Young's inequality

$$\|\sum_{p\in D_0} W^p + \sum_{p \in D_p} W^p\|^2_{L^2(U)} \leq C\left(\|\sum_{p\in D_0} W^p\|^2_{L^2(U)} + \|\sum_{p\in D_p} W^p\|^2_{L^2(U)}\right) \tag{5.3}$$

where the constant does not depend on the cardinality of each sum, and the two vector fields on the right hand side consist of fields with disjoint support. The bounds easily follow as in the previous two proofs. Suppose now that $D_s \neq \varnothing$. We follow the procedure outlined above for paired defects and holes of fields with localised curl. For the set D_s we define the Poisson equations

$$\begin{cases} -\Delta u^p = f^p := f\chi(B_r(p)), p \in D_s \end{cases}$$

There is no way to truncate these fields as they possess circulation. We therefore define $W^p = \nabla u^p J$ globally. Consider

$$W = \sum_{p\in D_0} W^p + \sum_{p\in D_p} W^p + \sum_{p\in D_s} W^p,$$

where W_p is defined as in the previous proof for all paired or screened defects. We then have

$$\|W\|^2_{L^2(U)} \leq 2\|\sum_{D\setminus D_s} W^p\|^2_{L^2(U)} + 2\|\sum_{p\in D_s} W^p\|^2_{L^2(U)}.$$

and apply the same inequality (5.3) as in the case of $D_s = \varnothing$ again to the rightmost term. Lemmas 7.0.3, 7.0.4, and 7.0.2 yield

$$\|\sum_{p\in D_0} W^p\|^2_{L^2(U)} = \sum_{p\in D_0} \|W^p\|^2_{L^2(B_{2\alpha}(p))} \leq \alpha C(r_m)\|f\|^2_{L^2(N_\alpha(D_0))}.$$

$$\|\sum_{p\in D_p} W^p\|^2_{L^2(U)} = \sum_{p\in D_p} \|W^p\|^2_2 \leq rC(r_m) \sum_{(x,y)\in D_p} \log|x-y|f\|^2_{L^2(N_r(x,y))},$$

$$\|\sum_{p\in D_s} W^p\|^2_{L^2(U)} \leq Cr|D_s| \sum_{p\in D_s} \|W^p\|^2_2 \leq Cr|D_s| \log \operatorname{diam}(r^{-1}U)\|f\|^2_{L^2(N_r(D_s))},$$

whence

$$\|W\|^2_{L^2(U)} \leq E(f)^2.$$

$\square$

Proof of Corollary 5.6.3. Take $|D| = 1$ and $r = \operatorname{diam}(U)$ in the above. Solving Poisson's equation with RHS equal to the curl of V yields a vector field with curl supported in a ball of diameter equal to the diameter of U for which the inequality found in the discussion above can be used. $\square$

5.8 Rigidity for Admissible Deformation Fields

We now prove a rigidity estimate that applies to the admissible configurations of section 2.12. It uses the fact that admissible configurations yield admissible vector fields, along with the lower bounds for non-linear defect energies, in particular that of Equation (4.10).

Lemma 5.8.1 (Rigidity for Admissible Configurations)**.** *Let $\omega \in \Omega_n$. For any local deformation field V^ω there exists a constant rotation R and vector field $\gamma^\omega \in L^2(\cup T^\omega, \Gamma)$ such that*

$$\|V^\omega - \gamma^\omega R^\omega\|^2_{L^2(\cup T^\omega)} \leq C(U_1)\|\mathrm{dist}(V, \mathrm{SO}(2))\|^2_{L^2(\cup T^\omega)} + C(V)r^2|D|.$$

where the constants do not depend on n but only model parameters.

Proof. Since ω is admissible there is some admissible vector field $\gamma^\omega V^\omega$ that is locally a gradient on $\cup T^\omega$ with an extension to U_n, the extension of which is an admissible vector field $\tilde{V}^\omega \in A_{r,\alpha}(U_n)$ for some choice of constants that only depend on the model. Let W_0 be the vector field generated through Poisson's equation for the screened defects as in the proof of Theorem 5.6.1. Around each individual defect in D_p, $\gamma^\omega V^\omega$ has a non-trivial Burgers vector in the annulus $A_{\frac{\rho}{2},\alpha_p}$. By Lemma 4.7.1 there exists a constant $C(A_{2,1})$ such that

$$\|\mathrm{dist}(\gamma^\omega V^\omega - W_0, \mathrm{SO}(2))\|^2_{L^2(A_{\frac{\rho}{2},\alpha_p})} \geq C\|\operatorname{curl}\tilde{V}^\omega\|^2_{B_{\alpha_p}} \log\frac{\rho}{2}$$

since $\sup_{\omega\in\Omega_n}|\operatorname{curl}\tilde{V}^\omega|_\infty \leq \infty$. The constant does not depend on the interior defect size due to Theorem 4.4.1. Note that since there could be other non-trivial Burgers vectors in the ball $B(x,\rho)$ the contour integral in the inequality (4.9) cannot be bounded below by only the "unbound" defect contained by $B(x,\alpha_p)$. However, it can be applied to the difference above. Applying the rigidity estimate for an $r-$localised vector field with $D_s = \varnothing$ and the pairing D_p in Theorem 5.4.1 yields the existence of a rotation $R \in \mathrm{SO}(2)$ such that

$$\begin{aligned}\|\gamma^\omega\tilde{V}^\omega - R^\omega\|^2_{L^2(U_n)} &\leq C(U_n)\|\mathrm{dist}(\tilde{V}^\omega, \mathrm{SO}(2))\|^2_{L^2(U_n)}\\ &\quad + C\left(\alpha_0\|\operatorname{curl}\tilde{V}^\omega\|^2_{N_r(D_0^\omega)} + \alpha_p\sum_{(x,y)\in D_p^\omega}\|\operatorname{curl}\tilde{V}^\omega\|_{N_r(x,y)}\ln|x-y|\right).\end{aligned}$$

Since $C(\rho) \geq \mathrm{dist}(x,y) > \rho$ for all $(x,y) \in D_p^\omega$ and fixed constants we have

$$\begin{aligned}
\|\gamma^\omega V^\omega - R^\omega\|^2_{L^2(\cup T^\omega)} &\leq C(U_n)\|\mathrm{dist}(\tilde{V}^\omega, \mathrm{SO}(2))\|^2_{L^2(U_n)} \\
&+ C_1\alpha_0\|\operatorname{curl}\tilde{V}^\omega\|^2_{N_r(D_0^\omega)} + C_2\alpha_p \sum_{(x,y)\in D_p^\omega} \|\operatorname{curl}\tilde{V}^\omega\|_{N_r(x,y)} \ln\rho \\
&\leq C(U_1)\|\mathrm{dist}(V^\omega, \mathrm{SO}(2))\|^2_{L^2(U_n)} + C(V)|D_0^\omega| + \\
&+ C(A_{2,1}) \sum_{x\in D_p^\omega} \|\mathrm{dist}(V^\omega, \mathrm{SO}(2))\|^2_{L^2(B_{\frac{1}{2}\rho}(x))} + \|W_0\|^2 \\
&\leq (C(U_1) + C(A_{2,1}))\|\mathrm{dist}(\tilde{V}^\omega, \mathrm{SO}(2))\|^2_{L^2(U_n)} + C(V)|D_0^\omega|.
\end{aligned}$$

Recalling the estimates on the vector field W_0 and the maximum allowable defect sizes yields the final line. Finally, we have (changing γ to γ^T and noting that $|\mathrm{dist}(\tilde{V}^\omega, \mathrm{SO}(2))|$ is also uniformly bounded in ω) that

$$\|V^\omega - \gamma^\omega R^\omega\|^2_{L^2(\cup T^\omega)} \leq C(U_1)\|\mathrm{dist}(V^\omega, \mathrm{SO}(2))\|^2_{L^2(\cup T^\omega)} + C(V)|D|.$$

□

This will ultimately be the class of defects and the rigidity estimate we use to demonstrate the main result in the next chapter. As a reminder, note that the above allows for configurations with defect pairs $(x,y) : \mathrm{dist}(x,y) \propto n$, as long as the number of dipoles (additional to screened clusters) in this configuration is of $O(1)$. That is admissible configurations are made up of defects that screen each other at one uniformly fixed length scale α as well as some other $\omega-$ dependent length scale $\rho(\omega)$, which can scale with system size.

Chapter 6

Statistical Mechanics

We now return to the task introduced in Chapter 1, to quantify the ordering of a thermalised system of atoms. To begin with we provide a brief review of why the ground state of such a system should be a periodic structure in the first place.

In the context of analysis, the fact that ordered configurations of points are preferred by various energy functionals is well studied. Indeed the triangular lattice, or appropriate transformations thereof, is known to minimise various energy functionals on finite or countable sets of points in the plane (Bétermin and Zhang [2014], Bourne et al. [2012], Theil [2006]). These energies, in particular, are invariant under a uniform shift or rotation of every point in a given configuration.

So while an energy has a *continuous symmetry group*, its minimiser (the lattice) has a discrete symmetry group. Performing transformations such as rotations will give a configuration with the same energy, these configurations can be distinguished from each other. We say the triangular lattice possesses order, because it has a smaller (but non-trivial) symmetry group relative to the energy it is a minimiser of.

The idea of studying the existence or non-existence of ordering in low dimensional, thermalised atomistic systems goes back to Mermin in Mermin [1968]. A system of atoms interacting through a Leonard-Jones type pair potential at finite temperature was considered. The first difficulty is to actually define what is meant by order. A strict definition of *crystalline order* is given, and it is shown that there is no finite temperature for which a "large" crystal exhibits this ordering property.

However in Mermin [1968] (remark (d) concerning the main result), a possible exception is discussed. At least for a lattice model with harmonic interactions, a weaker *orientational ordering* is present at low temperature.

Let e denote the edge joining $(0,0)$ to $(1,0)$ in the triangular lattice. In the notation from the introduction it is shown in Mermin [1968] that the correlations

$$\mathbb{E}_{\sigma,\beta,n}[(u^{\omega}(ne) - u^{\omega}((n-1)e)) \cdot (u^{\omega}(e) - u^{\omega}(0))] > 0,$$

for arbitrary n (see also Peierls [1979]). In fact, it can be shown this result is present in the model of Heydenreich et al. [2014], and is a consequence of the fact that

$$\limsup_{n\to\infty} \lim_{\beta\to\infty} \mathbb{E}_{\sigma,\beta,n}[\|\nabla u^{\omega} - I\|^2_{L^2(U_n)}] = 0.$$

The above result is shown in (1.1). It is also shown that as a consequence of this, the equality

$$\lim_{\beta\to\infty} \limsup_{n\to\infty} \sup_{t\in T_n} \mathbb{E}_{\sigma,\beta,n}[|\nabla u^{\omega}(t) - I|^2] = 0,$$

holds. It is possible to write, using $(u^{\omega}(ne) - u^{\omega}((n-1)e)) := Du^{\omega}_n$ as shorthand,

$$Du_n \cdot Du_0 = (\nabla u^{\omega}_n e) \cdot \nabla u_0 e$$

and noticing that $\sup_t |\nabla u^{\omega}(t) - I| < \delta$ for large enough β for given small δ. Performing some algebra and leveraging bounds in Heydenreich et al. [2014] yields the claim. The exact steps are not the focus of this thesis as we instead work with the generalised orientational ordering from the introduction. We merely point out that for simple models, there is a way to transition between these two definitions of orientational ordering, although the integral form is a weaker statement for other defects as mentioned in the introduction.

This weaker idea of ordering has been studied in many different contexts. In Aumann [2015] and Heydenreich et al. [2014] showed that tools from plasticity theory (Aumann [2015],Friesecke et al. [2002],Müller et al. [2014]) can be used to demonstrate analogues of this result. These generalisations hold in both in a lattice model of a crystal at finite temperature β^{-1} and a more general model based on a point process instead of a reference configuration, though the latter comes with problematic restrictions. We now introduce the model that we couple our admissible configurations to and to which improved rigidity estimates apply. We also prove some results regarding more general configurations introduced below.

6.1 Regular Configurations and Hamiltonian

To begin with we define an energy on finite point configurations as in Aumann [2015]. Collect into $\tilde{\Omega}_n$ the configurations $\omega \subset U_n$ that satisfy:

- $|T^\omega| \geq c_0|U_n|$ for some c_0
- The restricted tiling T^ω (which we now just call a tiling, as we do not use the unrestricted one), in addition to being connected and locally lattice-like by construction, is ρ-regular for some fixed ρ.
- Defects have both a minimum and maximum size ρ_1, ρ_2 respectively.

We define the Hamiltonian by

$$H(w) = \sum_{t \in T^\omega} H_l(t) + \sigma|\partial D^\omega| + \tau|v(T^\omega)^c|,$$

where the $H_l(t) : N_\epsilon(t_0) \to \mathbb{R}_+$ are continuous, rotationally invariant *local Hamiltonians.* $\sigma > 0$ is some parameter which punishes all configurations for which $D^\omega \neq \varnothing$.

The term $|\partial D^\omega|$ is the number of edges belonging to the *interior boundary* of the tiling (c.f. Chapter 2). Previously in models such as the one analysed in Heydenreich et al. [2014] the number of defects was punished. These were point defects, but as mentioned in Chapter 2 we work with vector fields with an underlying fixed length scale of order 1. Due to the minimum defect size we enforce punishing the perimeter of defects is more natural. However since we also enforce a maximum defect size, tiling regularity, and that an edge length must lie between $1 - \epsilon$ and $1 + \epsilon$, it is easy to see the cardinality $|\partial D^\omega|$ is comparable to the number of disjoint individual defects contained within D^ω, as each defect has a fixed maximum and minimum perimeter in this model.

Finally $\tau > 0$ punishes configurations with $v(T^\omega)^c \neq \varnothing$. This is the set of points in ω that are not vertices of any tile- they represent interstitial defects. We will assume that the local Hamiltonians satisfy

$$H_l(t) \geq C\|\mathrm{dist}(\nabla v_t, \mathrm{SO}(2))\|^2_{L^2(t)},\ H_l(t) = 0 \text{ for } t \in N_0(t_0).$$

for a piecewise affine local deformation of a tile given in Chapter 2. As in that section this object is not unique, however the lower bound is the same in all four cases due to the rotational invariance of H_l. From the above considerations, we find that $H(\omega) = 0$ if and only if $\omega = \mathbb{Z}_n^2$ up to some translation due to the periodic boundary conditions. We define for the reference measure μ on $\tilde{\Omega}_n$, an appropriate

Poisson measure (see Aumann [2015]) the partition function

$$\tilde{\mathbb{P}}_{\sigma,\beta,n}(d\omega) = \tilde{Z}^{-1}_{\sigma,\beta,n} e^{-\beta H(\omega)} \mu(d\omega), \;\; \tilde{Z}_{\sigma,\beta,n} = \int_{\tilde{\Omega}_n} e^{-\beta H(\omega)} \mu(d\omega),$$

and we also define, when using only the admissible configurations $\Omega_n \subset \tilde{\Omega}_n$

$$\mathbb{P}_{\sigma,\beta,n} = Z^{-1}_{\sigma,\beta,n} e^{-\beta H(\omega)} \mu(d\omega), \;\; Z_{\sigma,\beta,n} = \int_{\Omega} e^{-\beta H(\omega)} \mu(d\omega).$$

We now discuss the main result of the thesis as well as results concerning the large-volume behaviour of $n^{-2}\tilde{\mathbb{E}}_{\sigma,\beta,n}[H(\omega)]$.

Theorem 6.1.1 (Uniform Orientational Ordering). *1.6.1 There exists $\sigma_0 \in \mathbb{R}_+$ which depends only on model parameters (not n or β) such that for all $\sigma > \sigma_0$*

$$\lim_{\beta\to\infty} \limsup_{n\to\infty} \; \mathbb{E}_{\sigma\beta,n} \left[\inf_{R\in SO(2)} \frac{1}{|T^\omega|} \sum_{t\in T^\omega} \|V^\omega - \gamma^\omega R^\omega\|^2_{L^2(t)} \right] = 0.$$

where $V^\omega \in L^2_{sym}(\cup T^\omega)$ is any choice of local deformation field *for each configuration, defined in Chapter 4, with $\gamma \in L^2(\cup T^\omega, \Gamma)$.*

Since we use periodic boundary conditions, the net Burgers vector of any configuration will be zero, making the set $D_s = \varnothing$ a.s. using the vector field description of a configuration. In addition to including defects that screen each other over a fixed length scale (the screening parameter α in our model), our results also allow for the presence of defects, mutually spaced over any length scale $s(\omega)$, that also screen each other over this length scale. An obvious target for future work is to bridge the gap between these two regimes. Rotational defects currently be included as an object whose ordering we can quantify. However, as in the discussion of discrete symmetry of a crystal, we have restored their status as a point defect in this framework and begun the process of adequately describing their behaviour through rigidity estimates. We can demonstrate some results regarding the expectation of the energy density even in this case, as well as offer some heuristic discussion later.

Lemma 6.1.2 (Large volume behaviour of the energy). *For the configuration space $\{\tilde{\Omega}_n\}_{n\geq 1}$,*

$$\limsup_{n\to\infty} \tilde{\mathbb{E}}_{\sigma,\beta,n}[H(\omega)] := e(\beta)$$

exists for all $\beta > \beta_0$ where β_0 depends only on model parameters. Moreover, $e(\beta) \to 0$ as $\beta \to \infty$.

Remarks. This allows us to control the energy of the system in the large n-limit even in the presence of rotational defects or dislocation dipoles that do not possess the mutual separation condition found in the definition of Ω_n. However the inequality needed to compare the order of a system to $e(\beta)$, either by extension of vector fields in $L^2_{sym}(\cup T^\omega)$ to U_n or other methods to control rigidity constants, is currently an open problem.

6.2 Proof of Theorem 1.6.1

This proof proceeds in two parts. We use the inequality found in Lemma 5.8.1 to relate the order of the system to its energy. Lemma 6.1.2 can then be applied to deduce the main result. This lemma relies on a lower bound of the partition function found in Lemma 3.1.1 of Aumann [2015]. As previously mentioned, we have removed the need for a global rigidity estimate to establish the behaviour of $\mathbb{E}[H(\omega)]$, laying the groundwork for future generalisations.

6.2.1 Comparing Order to Energy

Bounding the energy of a configuration from below by its order is an analytical exercise using the rigidity estimates established in previous chapters. Methods to bound expectations from Aumann [2015] can be used with these new estimates to produce the full result. We must show that for some fixed σ_0, for any $\sigma > \sigma_0$, for every ω there is a rotation R^ω such that

$$H(\omega) \geq C\|V^\omega - \gamma^\omega R^\omega\|^2_{L^2(\cup T^\omega)}.$$

for some choice of local deformation field $V^\omega \in L^2_{sym}(\cup T^\omega)$.Because $\cup T^\omega$ is a random domain, the constant in the rigidity estimate will not be the same for different configurations ω if we were to apply it to $\cup T^\omega$. Since ω has a consistent ordering, there is a means to choose γ^ω so that V^ω is curl-free on $\cup T^\omega$. We are able to demonstrate the following result, a variant of the result of Lemma 3.7 in Aumann [2015]. In contrast to the inequality of Lemma 3.7 the following estimate is independent of n. We have however restricted ourselves to the admissible configurations defined previously.

Lemma 6.2.1. *For all $\sigma > \sigma_0$ where σ_0 depends on model parameters but not on n or β, for every admissible ω there exists a rotation R^ω and a choice of local* *deformations such that*

$$H(\omega) \geq C\|V^\omega - \gamma^\omega R^\omega\|^2_{L^2(\cup T^\omega)},$$

where C is a constant uniform in ω, depending on model parameters only.

Proof. The idea is that thanks to the fact that $\|V - R\|2_{L^2(D)}$ and $\|\mathrm{dist}(V, SO)\|^2_{L^2(D)}$ scale like $|D|$, and the defects have a maximum size α, we can choose some $\sigma(\alpha)$ to "mop up" these terms if we can relate the energy of the system with the right hand side of the rigidity estimate. We recall Lemma 5.8.1 For all admissible configurations, there exists a rotation R^ω such that for any choice of local deformation field $V^\omega \in L^2_{sym}(\cup T^\omega)$

$$\|V^\omega - \gamma^\omega R^\omega\|^2_{L^2(\cup T^\omega)} \leq C(U_1)\|\mathrm{dist}(V^\omega, \mathrm{SO}(2))\|^2_{L^2(\cup T^\omega)} + C(V)|D|,$$

which follows since for some $\gamma \in L^2(\cup T^\omega, \Gamma)$ the vector field $(\gamma^\omega)^T V^\omega$ has an extension $\tilde{V}^\omega$ to all of U_n courtesy of Aumann [2015] with $|\tilde{V}^\omega|_\infty, |\,\mathrm{curl}\,\tilde{V}^\omega|_\infty < M$ uniformly in ω. Recalling the form of Hamiltonian chosen it is easy to see that

$$\|V^\omega - \gamma^\omega R^\omega\|^2_{L^2(\cup T^\omega)} \leq CH(\omega) + (C(V) - \sigma)|D|.$$

where as discussed the constant $C(V)$ is fixed dependent on model parameters and the maximum screening range for clusters of defects only. By picking $\sigma > \sigma_0 = C(V)$ the bracketed term is positive, yielding for all admissible configurations that there is a random symmetrised rotation with

$$\|V^\omega - \gamma^\omega R^\omega\|^2_{L^2(\cup T^\omega)} \leq CH(\omega), \tag{6.1}$$

and the constant does not depend on system size thanks to scale invariance of the rigidity estimate. □

Remarks. Thanks to the assumptions on the defect sets and the behaviour of constants in the rigidity estimates established earlier, we avoid a situation in which

$$H(\omega) \geq \|V^\omega - R^\omega\|^2_{L^2(\cup T^\omega)} + |D^\omega|(\sigma - C(n)^2).$$

With the estimate for general vector fields $V \in L^2_{curl}(U_n)$, to follow this procedure for demonstrating orientational ordering, σ must grow as the system size does.

If we had proved a rigidity estimate using an L^p-estimate of the curl rather than L^2, the above lower bound for the Hamiltonian would be modified to the form

$$H(\omega) \geq \|V^\omega - R^\omega\|^2_{L^2(\cup T^\omega)} + |C(\sigma|D| - n^{4-\frac{4}{q}}|D|^{\frac{2}{q}})$$

as

$$C_2(U_n)\|\operatorname{curl} V\|^2_{L^q} \leq C(|V|_\infty)n^{4-\frac{4}{q}}|D|^{\frac{2}{q}}$$

as in Lemma 3.9 of Aumann [2015]. This would not allow us to consider a finite density of defects. If $|D| = \rho n^2$ for some $\rho < 1$, then we arrive at trying to balance

$$\sigma n^2 - Cn^{4-\frac{4}{q}}n^{\frac{2}{q}}$$

clearly there is no way to bound the right side below by 0 uniformly in n without setting $q = 2$. Doing otherwise results in non-uniform estimates, which it is our goal to avoid. Avoiding this trap is the key to demonstrating orientational ordering for a uniform set of model parameters, and this is the case for the admissible configurations described above. We now state a lemma, the proof of which is postponed until the next section, which allows us to prove the main theorem.

Lemma 6.2.2. *For all $\beta > \beta_0$ where β_0 depends on model parameters only, the limit*

$$\limsup_{n\to\infty} \mathbb{E}_{\sigma,\beta,n}[n^{-2}H(\omega)] := e(\beta)$$

exists, and moreover $\lim_{\beta\to\infty} e(\beta)=0$*.*

The main result of this thesis, Theorem 1.6.1 is a direct consequence of these lemmas. We provide the final lines for completeness and to benefit a heuristic discussion on rotational defects later.

Proof of Main Theorem. We take the expectation of the inequality (6.1) and rewrite the integrals as sums over tile integrals to find

$$\begin{aligned}\mathbb{E}_{\sigma,\beta,n}\left[\inf_{R\in SO(2)} \frac{1}{|T^\omega|}\sum_{t\in T^\omega}\|V^\omega - \gamma^\omega R\|^2_{L^2(t)}\right] &\leq C|T^\omega|^{-1}\mathbb{E}_{\sigma,\beta,n}\left[H(\omega)\right]\\ &\leq Cn^{-2}\mathbb{E}_{\sigma,\beta,n}\left[H(\omega)\right]\end{aligned}$$

where the rightmost inequality is due to the connectivity of T^ω and the minimum defect separation yielding the inequality $|T^\omega| \geq c_0|U_n|$. Lemma 6.2.2 yields that

$$\lim_{\beta\to\infty}\limsup_{n\to\infty}\mathbb{E}_{\beta,n}[H(\omega)] = 0,$$

and so the main theorem follows by taking the two limits in the correct order. $\square$

6.3 Large Volume Bound of the Energy

The goal of this section is to examine the existence and behaviour of

$$\tilde{e}(\beta) = \limsup_{n\to\infty} n^{-2}\tilde{\mathbb{E}}_{\sigma,\beta,n}[H(\omega)] = \tilde{Z}^{-1}_{\sigma,\beta,n} \int_{\tilde{\Omega}_n} e^{-\beta H(\omega)} d\mu, \tag{6.2}$$

where $\tilde{\Omega}_n$ consists of all configurations matching the conditions in Section 6.1. The end result of this section constitutes the proof of Lemma 6.1. The main improvements made here over existing results is that we allow for configurations with no consistent ordering rigorously, as well as any configuration of defects that meets some spacing and sizing assumptions. This result therefore applies to a broader class of configurations than the admissible ones. The two main ideas in proving Lemma 6.1 are that the rigidity estimate can be applied locally. This gives us a lower bound on the energy in terms of the square of distances of points in the configuration ω after an appropriate change of variables. From this, we can bound the integrand in (6.2) by a system of Gaussian integrals. This is a commonly used method in statistical physics. We begin by establishing some notation in a similar way to Aumann [2015], though the full details of an appropriate lower bound on $H(\omega)$ as in Lemmas 3.12 and 3.13 differ.

6.3.1 Configurations and Graphs

In a similar way to Lemma 3.12 of Aumann [2015], we will bound the full energy of the Hamiltonian from below by only looking at the contribution from some specific edges, multiplied by an appropriate constant. This provides a bound above on the expectation of the energy, with is further bounded above by enlarging the state space to allow points to lie at any distance from each other. This multi-dimensional integral can be computed exactly and compared with an appropriate lower bound on the partition function from Aumann [2015]. To this end, we define $E(T^\omega)$ to be the edges of the tiling of ω and recall the notation for its vertices $v(T^\omega)$. We then consider the graph $G(\omega) = (v(T^\omega), E(T^\omega))$. This is a connected graph by assumption, whence it possesses a spanning tree $\mathcal{T}(G(\omega))$ (c.f. Flajolet and Sedgewick [2009]). A spanning tree is a sub-graph of G containing all its vertices and a minimal number of edges.

This tree can be labelled by an appropriate index set $I = \{1, ..., |v(T^\omega)| := m\}$. As it is a tree it has $m-1$ edges in total. The tree can be labelled so that a point k always shares an edge with point $k-1$ for all $k > 1$. This can be done by labelling points on the same level of the tree consecutively, then moving down to the next level once these are exhausted. This allows an enumeration of points $X_k \in v(T^\omega) : k \in 1, \dots, m$. We use this labelling of points to produce a labelling of edges $E(\mathcal{T}) = \{e_1, e_2, ..., e_{m-1}\}$ such that consecutive edges e_k, e_{k+1} share the point X_k.

Lemma 6.3.1. *For all $\omega \in \tilde{\Omega}_n$, there exists some spanning tree $\mathcal{T}$ such that for any choice of local deformation field $V^\omega \in L^2_{sym}(\cup T^\omega)$, and for the point and edge labelling as above,*

$$H(\omega) \geq C \sum_{k=1}^{m-1} |\xi_k - (X_k - X_{k+1})|^2 - cm$$

where $\{X_k\} : k = 1, \cdots, |v(T^\omega)| := m$ are the points in the tiling, c, C depend on model parameters but not T^ω, and $\xi_k \in \mathbb{R}^2$ are a set of vectors fixed for the spanning tree $\mathcal{T}$ and the same for each T^ω with this tree.

Proof. We need only the local rigidity estimate on every tile t: for any choice of local deformation for a tile there exists a fixed rotation such that

$$\|\mathrm{dist}(V^\omega, \mathrm{SO}(2))\|^2_{L^2(t)} \geq C(t)\|V^\omega_t - R_t\|^2_{L^2(t)}.$$

Since the tile size and maximum strain is uniformly bounded, these domains have a uniformly bounded rigidity constant, allowing us to take the infimum over all individual tiles to yield for a fixed constant that

$$\|\mathrm{dist}(V^\omega, \mathrm{SO}(2))\|^2_{L^2(t)} \geq C(\epsilon)\|V^\omega_t - R_t\|^2_{L^2(t)}.$$

In fact the constant will depend on the $W^{1,\infty}$ norm of the piecewise affine bijections used from t_0 to tiles $t \in N_\epsilon(t_0)$, which has a fixed maximum due to the maximal strain condition. We now use this to bound the energy of configurations below using the notation developed above. Following Aumann [2015] we restrict the sum over all tiles in the following way:

$$\sum_{t \in T^\omega} H_l(t) \geq c(\epsilon)\|V_t - R_t\|^2_{L^2(t)} = \frac{c}{|v(t_0)|} \sum_{\text{edges of } t} |V_t - R_t|^2.$$

Now let the corners of a tile be denoted $X_1, ..., X_c$, in an anti-clockwise fashion. Since any tile has finite strain these have bounded minimum and maximum separation, whence

$$
\begin{aligned}
H_l(t) &\geq C \sum_{k \in v(t)} |V_t - R_t|^2 |X_{k+1} - X_k|^2 \\
&\geq C \sum_k |V_t(X_{k+1} - X_k) - R_t(X_{k+1} - X_k)|^2 \geq C \sum_k |R_t^T(\lambda^\omega) - (X_{k+1} - X_k)|^2 \\
&:= C \sum_k |\xi_k^\omega - (X_{k+1} - X_k)|^2.
\end{aligned}
$$

While not addressed in Aumann [2015], in fact the R_t depend on ω as do the $\lambda\omega$ (as they depend on the choice of local deformation field). We introduce $\xi^\omega = R_t^T$. In fact each ξ^ω is some rotation of a random vector of the ground state lattice thanks to the properties of V^ω. For each spanning tree we introduce an arbitrary set of vectors $\xi_k, k \in 1, \dots m-1$ such that $|\xi_k| \leq 1$. We then have that for all ω with the same spanning tree that

$$
H_l(t) \geq C \sum_{k=1}^{|v(t)|-1} |\xi_k - (X_{k+1} - X_k)|^2 - c_2|v(t)|,
$$

with c_2 some fixed constant and K the number of edges that we sum over, since the difference $|\xi_k - R_t^T \lambda_k^\omega| \leq c_2$ for all ω. Evidently the sum can be further restricted to only sum over a particular set of edges of our choosing then added together to result in the result of Lemma 6.3.1. □

6.3.2 Gaussian Integration

We now state the following lemma from Aumann [2015], where it is labelled Lemma 3.14. The overall result is obtained by splitting configurations up into the sets $\Omega_\delta = \{\omega : H(\omega) > \delta n^2\}$ and its complement. A lower bound on the partition function to integrate only over a subset of defect-free configurations. An upper bound on the un-normalised integral introduced below then yields the appropriate bound on $\tilde{E}[H(\omega)]$.

Lemma 6.3.2 (Bound on $e(\beta)$, Aumann [2015])**.** *Suppose the bound*

$$
\int_{\tilde{\Omega}_n} e^{-\beta H(\omega)} d\mu \leq c_1 e^{-n^2(\log\beta + c_2)} \tag{6.3}
$$

can be established for some $c_1 > 0, c_2 \in \mathbb{R}$. If the set $\Omega_0 = \{\omega : D^\omega = \varnothing\}$ is such that $\Omega_0 \subset \tilde{\Omega}_n$,

$$\lim_{\beta\to\infty} \limsup_{n\to\infty} n^{-2}\mathbb{E}_{\sigma,\beta,n}[H(\omega)] = 0.$$

.

Proof. See Aumann [2015]. □

Lemma 6.3.3. *Equation* (6.3) *holds for $\tilde{\Omega}_n$, and we may replace $\tilde{\Omega}_n$ by Ω_n in the result.*

Proof. The fact that the inequality and limit above hold for the admissible configurations since defect free configurations are admissible, and $\Omega_n \subset \tilde{\Omega}_n$ allowing us to bound the integral over Ω_n by the left hand side of (6.3). We therefore consider $\tilde{\Omega}_n$ WLOG in the following. Define the sets

$$\Omega(m, \mathcal{T}) = \{\omega \in \tilde{\Omega}_n : \cup T^\omega \text{ has the spanning tree } \mathcal{T}, |v(\mathcal{T})| = m\},$$

and note $\tilde{\Omega}_n = \cup_{\mathcal{T}} \cup_m \Omega(\mathcal{T}, m)$. Fix some m. We have that

$$\int_{\omega\sim\mathcal{T}} e^{-\beta H(\omega)} \leq e^{c_1 m} \int_{\omega\sim\mathcal{T}} e^{-C\beta\sum_{k=1}^{K}|\xi_k^{\mathcal{T}}-(X_{k+1}-X_k)|^2} d\mu,$$

by Lemma 6.3.1. We note that since for a fixed cardinality the points X_k are uniformly distributed over the box

$$\int_{\omega\sim\mathcal{T}} e^{c_1 m} e^{-C\beta\sum_{k=1}^{K}|\xi_k^{\mathcal{T}}-(X_{k+1}-X_k)|^2} d\mu \leq 1 \cdot C^m n^{-2m} \int_{U_n^m} e^{-C\beta\sum_{k=1}^{K}|\xi_k^{\mathcal{T}}-(X_{k+1}-X_k)|^2} \prod_k dX_k.$$

where the 1 term is the integration over interstitial points for each configuration. We wish to diagonalise this to produce a product of Gaussian integrals. Since we have removed the ω-dependence of the $\xi_k^{\mathcal{T}}$ for each tree we may perform a change of variables, and further expand the integration from U_n^m to $\mathbb{R}^{2m}$. For this we define the following matrix $M_{\mathcal{T}}$.

$$M_{\mathcal{T}}(i,j) = \begin{cases} -2 \text{ if } X_j \sim X_i, \;\; j < i \\ \#X_j : X_j \sim X_i, \;\; i = j. \\ 0, \;\; j > i \end{cases}$$

All entries above the lead diagonal are 0 rather than choosing -1 of both off-diagonals in order for us to evaluate the determinant. Now, let $\zeta_k = (M_{\mathcal{T}}X - \xi)_k$.

The matrix M is such that $|M_{\mathcal{T}}X - \xi|^2 = \sum_{e\in E(\mathcal{T})} |X_{k+1} - X_k - \xi_k^{\mathcal{T}}|^2$. This is seen by inspection. The lead diagonal of $M_{\mathcal{T}}$ is not one because points would be under-counted. To appropriately produce the right numbers it needs to equal the connectivity of each X_i. Because of this and the lower triangular form of $M_{\mathcal{T}}$, $\det M_{\mathcal{T}} = \prod_i M_{\mathcal{T}}(i,i) \leq c_{\mathbb{Z}^2}^m$ (c.f. Bronson [2014]). Here c is maximum number of neighbours of a point X. Because tiles have a bounded upper and lower size, this is finite constant irrespective of system size n, depending only on model and reference tiling parameters. Combining the above yields

$$\int_{\omega\sim\mathcal{T}} e^{-\beta H(\omega)} \leq n^{-2m}(\det M_{\mathcal{T}})c^m \left(\int_{\mathbb{R}^2} e^{-C\sum_{k=1}^{m-1}\beta|\zeta_k|^2}\right) d\zeta \leq C^m n^{-2m}\beta^{-m}.$$

for some fixed constant C depending only on model parameters. We now appeal to Cayley's formula (found e.g. in Flajolet and Sedgewick [2009]) and the minimum and maximum numbers of m attainable for such configurations as in Aumann [2015]. Due to the minimum size $|T^\omega| \geq c_0|U_n|$ and the maximum density of a tiling at any point, we find constants a, b so that $\Omega(m,\mathcal{T}) = \varnothing$ if $m \notin [an^2, bn^2]$. We arrive at

$$\begin{aligned}\int_{\tilde{\Omega}_n} e^{-\beta H(\omega)} &\leq \sum_{m=an^2}^{bn^2} |\mathcal{T}_m| C^m n^{-2m}\beta^{-m} \\ &\leq \sum_m m^{-2} m^m n^{-2m} e^{-m(\log\beta - C_{\mathbb{R}})} \\ &\leq e^{-an^2(\log\beta - C_{\mathbb{R}})} \sum_m m^{-2} m^m n^{-2m} \leq e^{-an^2(\log\beta - C_{\mathbb{R}})}.\end{aligned}$$

□

Proof of Lemma 6.1.2. With this estimate we may use a result by Aumann [2015]: Employing the result of Lemma 6.3 noting it holds for $\Omega_n, \tilde{\Omega}_n$ by Lemma 6.3.3 we arrive at (taking the expectation over either set)

$$\lim_{\beta\to\infty} \limsup_{n\to\infty} \mathbb{E}_{\sigma,\beta,n}[H(\omega)] = 0,$$

□

6.4 Heuristics: Energy of Rotational Defects

While we do not have an extension theorem for locally Curl-free vector fields (vector fields with a Frank vector) and so cannot produce a rigidity estimate for non-trivial symmetrised fields on a simply connected domain, it is known in the literature that they have a very large energy compared to dislocations (e.g. Kostorz et al. [2013], p64), and heuristically the estimate in Chapter 4 supports this. We do not expect to see "large" disclinations or disclination dipoles appear in this model a priori. It should be possible to demonstrate

$$\mathbb{P}_{\sigma,\beta,n}(\text{disclination length} > \rho n) \leq \mathbb{P}_{\sigma,\beta,n}(H(\omega) \geq \rho n^2) \lesssim \frac{1}{\rho} n^{-2}\mathbb{E}_{\sigma,\beta,n}[H(\omega)]$$

. where the last inequality can be bounded above using Lemma 6.1.2. While we do not have a rigidity estimate to yield the existence of particular rotations to compare order to energy, we find since $|V^\omega|_\infty < M$ uniformly

$$\begin{aligned}
&n^{-2}\mathbb{E}_{\sigma,\beta,n}[\min_{R\in \mathrm{SO}(2)} \|V^\omega - \gamma^\omega R\|^2] \leq \\
&n^{-2}\mathbb{E}_{\sigma,\beta,n}[\|V - \gamma^\omega R\|^2|\gamma_F = I] + C(V)\mathbb{P}_{\sigma,\beta,n}[|\text{disclinations}| > 0]
\end{aligned}$$

and so the rightmost term can be controlled a priori for large disclination dipoles, with the first term being controlled with rigidity. Since dislocation dipoles have an energy proportional to $\log n$ this argument cannot be used for them. Formally, both disclinations and dislocations are point defects they should have the same entropy. A statement of the form

$$\mathbb{P}_{\sigma,\beta,n}(\text{disclination dipole}) = o(\mathbb{P}_{\sigma,\beta,n}(\text{dislocation dipole})).$$

should be available with more work on the statistics of these configurations due to their energy differences. This is a first step to showing that configurations consisting of dislocation dipoles make up a much larger share of the partition function than disclinations. Assuming a justification of the lower bound on disclination energy (c.f) we could at least demonstrate orientational ordering when a dilute set of large disclination dipoles are allowed into the model. While we cannot currently compare their order to energy, we can control of the expectation of the Hamiltonian in the presence of disclinations.

Chapter 7

Bounds for Solutions to Poisson's Equation

We are interested in the properties of solutions to Poisson's equation in the plane,

$$\begin{cases} -\Delta u = f, \\ f \text{ is compactly supported and } f \in L^2(\mathbb{R}^2). \end{cases}$$

Of course while solutions are not unique, we will only need the solution

$$u(x) = C \int_{\mathbb{R}^2} \Phi(|x-y|) f(y) dy, \quad \Phi(t) := \log(t), \ t \geq 0. \tag{7.1}$$

The L^2 regularity of this solution and its partial derivatives is the limiting factor in improving the rigidity estimates found in the main results. In this section we state and prove some lemmas that are used to produce the right hand side of the rigidity estimate. For references on the results used in this section see Tikhonov and Samarskii [2013], Cerda [2010], and Kreyszig [2007].

Lemma 7.0.1 (Logarithmic Bound for Poisson's Equation)**.** *Let U be a bounded, Lipschitz domain with $0 \in U$ and let $f \in L^2(B_r(0))$. Then the solution* (7.1) *to Poisson's equation with right hand side f has the property that*

$$\|\nabla u\|^2_{L^2(U)} \leq C r^2 \|f\|^2_{L^2(B_r(0))} \log(\operatorname{diam}(U)).$$

Lemma 7.0.2 (Multiple defects)**.** *Let U be a bounded, Lipschitz domain with $0 \in U$. Let $D \subset U$ be a finite set of points with* $\operatorname{dist}(x, y) > 2r$ *for some given $r > 0$. Moreover, suppose $f \in L^2(\cup_{x \in D} B_r(x))$. Then the solution to Poisson's equation* *with right hand side f has the property that*

$$\|\nabla u\|^2_{L^2(U)} \leq Cr^2 |D| \|f\|^2_{L^2(U)} \log(\mathrm{diam}(U)).$$

Lemma 7.0.3 (Integrable Solution To Poisson's Equation)**.** *Suppose that $f \in L^2(\mathbb{R}^2)$ is compactly supported,* $\mathrm{supp} f \subset B_r(0)$ *and that $\int f = 0$. Then for u defined component-wise as in equation 7.1, $u \in H^1(\mathbb{R}^2, \mathbb{R}^2)$. Moreover,*

$$\|D^\alpha u\|^2_{L^2(\mathbb{R}^2)} \leq Cr^2 \|f\|^2_{L^2(B_r(0))},$$

for $|\alpha| \leq 1$.

Lemma 7.0.4 (Paired Solution To Poisson's Equation)**.** *Let U be a bounded, Lipschitz domain with $0 \in U$. Let $x, y \in U$ with* $\mathrm{dist}(x, y) > 2r$ *for some given $r > 0$. Moreover, suppose $f \in L^2(\mathbb{R}^2)$,* $\mathrm{supp} f \subset B_r(x) \cup B_r(y)$ *and that*

$$\int_{B_r(x)} f = -\int_{B_r(y)} f.$$

Then $u \in H^1(\mathbb{R}^2, \mathbb{R}^2)$. Moreover,

$$\|D^\alpha u\|^2_{L^2(\mathbb{R}^2)} \leq Cr^2 \|f\|^2_{L^2(\mathbb{R}^2)} 1 \vee \log|x-y|,$$

for $|\alpha| \leq 1$.

7.0.1 Proofs of L^2-Regularity Lemmas

Proof of Lemma 7.0.1. The proof of this lemma is straightforward. We begin by considering partial derivatives of u. We assume WLOG that the defect is located at 0. Using the representation formula we have outside of $B_{2r}(0)$

$$\begin{aligned} |\partial_j u|^2 = \left| \int_{B_r(0)} f(y) \partial_j \Phi(x-y) dy \right|^2 &\leq \int_{B_r(0)} |f(y)|^2 dy \lambda(B_r) \cdot \frac{1}{\lambda(B_r)} \int_{B_r(0)} |\partial_j \Phi(x-y)|^2 dy \\ &\leq C\lambda(B_r) \|f\|^2_{L^2(B_{2r}(0))} \cdot \frac{1}{|x|^2}. \end{aligned}$$

We now integrate over $U \backslash B_{2r}(0)$ to obtain

$$\begin{aligned} \int_{U \backslash B_{2r}(0)} \left| \int_{B_r(0)} f(y) \partial_j \Phi(x-y) dy \right|^2 dx &\leq Cr^2 \|f\|^2_{L^2(B_r(0))} \int_{U \backslash B_{2r}(0)} \frac{1}{|x|^2} \\ &\leq Cr^2 \|f\|^2_{L^2(B_r(0))} \log(\mathrm{diam}(U)). \end{aligned}$$

For the region $B_{2r}(0)$, $\partial_i\Phi$ is not square-summable. We therefore apply Young's inequality to the formula for $\partial_i u$ to yield $\|\partial_i u\|_2^2 \leq \|\partial_i\Phi\|_1^2\|f\|_2^2 \leq Cr^2\|f\|_2^2$. We find

$$\|Du\|^2_{L^2(U)} \leq Cr^2\|f\|^2_{L^2(B_r(0))}1 \vee \log(\operatorname{diam}(U)).$$

□

Proof of lemma 7.0.2. With multiple defects we use superposition, the previous lemma, and Jensen's inequality. We find

$$|\partial_i u(z)|^2 = |D|^2 \left|\frac{1}{|D|}\sum_{x\in D}\int_{\mathbb{R}^2} f^x(y)\partial_i\Phi(z-y)dy\right|^2 \leq |D|\sum_{x\in D}\left|\int_{\mathbb{R}^2} f^x(y)\partial_i\Phi(z-y)dy\right|^2.$$

We now consider integrating individual terms in this sum. By Lemma 7.0.1 we have

$$\|(Du^x)\|^2_{L^2(U)} = \int_U\left|\int_{\mathbb{R}^2} f^x(y)\partial_i\Phi(z-y)dy\right|^2 dz \leq Cr^2\log\operatorname{diam}(U)\|f^x\|^2$$

by the previous lemma. Applying this and the above calculations to equation 7.0.1 we arrive at

$$\|Du\|^2_{L^2(U)} \leq Cr^2|D|\sum_{x\in D}\|f_x\|^2_{L^2}\log(\operatorname{diam}(U)) = Cr^2|D|\|f\|^2_{L^2}\log(\operatorname{diam}(U)).$$

Combining the above completes the proof. □

Proof of Lemma 7.0.3. For this proof and the next we will use Fourier methods. For any $\varphi \in S(\mathbb{R}^2)$ we have

$$((Du)_{ij},\varphi)_{L^2} = (\hat\Phi, -\widehat{\partial_i f_j * \varphi}) = (\hat\Phi, -k_i\hat f_j\hat\varphi).$$

We have

$$(\hat\Phi, -k_i\hat f\hat\varphi) = \int_{|k|\leq 1}\frac{k_i\hat{\varphi(k)}\hat f_j(k)}{|k|^2} + \int_{|k|>1}\frac{k_i\hat\varphi(k)\hat f_j(k)}{|k|^2} + C\cdot 0.$$

Using the triangle inequality we consider these terms separately.

$$|(\hat\Phi, -k_i\hat f\hat\varphi)| \leq \left|\int_{|k|\leq 1}\frac{k_i\hat{\varphi(k)}\hat f_j(k)}{|k|^2}\right| + \left|\int_{|k|>1}\frac{\hat\varphi(k)\hat f_j(k)}{|k|^2}\right| \leq I_1 + I_2,$$

with

$$I_1 := \left| \int_{|k|\le 1} \frac{k_i \varphi(\hat{k}) \hat{f}_j(k)}{|k|^2} \right|, \; I_2 := \left| \int_{|k|>1} \frac{\hat{\varphi}(k)\hat{f}_j(k)}{|k|^2} \right|.$$

We bound I_1 first. We use the Cauchy Schwarz Inequality to split the product into one containing the L^2 norm of φ, and the second containing terms $k_i \hat{f}$. We have

$$|I_1|^2 \le \|\hat{\varphi}\|^2_{L^2(B_1(0))} \int_{|k|\le 1} \frac{|\hat{f}_j(k)|^2}{|k|^2} dk.$$

Taylor's theorem yields

$$\hat{f}_j = 0 + R_f \cdot k, \text{ near } 0$$

where $|R_f| \le \sup_{B_1(0)} |\nabla \hat{f}_j(\xi)|$. We now use that $\hat{f}$ is the Fourier transform of f to find

$$|\partial_i \hat{f}_j(k)|^2 = \left| \int_{B_r(0)} x_i f_j(x) e^{ik\cdot x} dx \right|^2 \le Cr^2 \left(\int_{B_r(0)} |f| dx \right)^2 \le Cr^2 \|f\|^2_{L^2(\mathbb{R}^2)},$$

with the last inequality reached by using Jensen's inequality. It follows that

$$\int_{|k|\le 1} \frac{|\hat{f}(k)|^2}{|k|^2} dk \le r^2 \|f\|^2_{L^2(\mathbb{R}^2)} \left(\int_{|k|\le 1} \frac{0 + |k|^2}{|k|^2} dk \right) \le Cr^2 \|f\|^2_{L^2(\mathbb{R}^2)}.$$

We bound $|I_2|$ by noting $|k| > 1$ in this region so we use the fact that $\hat{f} \in L^2(\mathbb{R}^2)$. Combining the above yields

$$|(\hat{\Phi}, -k_i \hat{f} \hat{\varphi})| \le C(r+1) \|\varphi\|_{\mathbb{R}^2} \|f\|_{L^2(\mathbb{R}^2)}.$$

It follows that $u \in H^1(\mathbb{R}^2)$. □

Proof of Lemma 7.0.4. We assume WLOG that f consists of a function supported in one ball and a translated 'mirror' in another, that is $f = \tilde{f}(x - x^0) - \tilde{f}(x - x^1)$. If this is not the case we add and subtract $f\chi(B_r(x^0))(x - x^0)$ to f. Then f is the sum of two functions: one has the required form, and the second is a function supported in $B_r(x^0)$ with $\int \operatorname{curl} f = 0$. We may then apply Lemma 7.0.3 to the latter and this proof to the former. We now continue with the lemma. Let $\varphi \in S$. We have that

$$(\partial_i u, \varphi) = (\Phi, -f * \partial_i \varphi) = (\hat{\Phi}, (\widehat{-f * \partial_i} \varphi)).$$

We first consider the transform of f, and take x^0 in the above representation of f to be the origin. We find

$$\int e^{ik\cdot x}(f(x) - f(x - x^1))dx = (1 - e^{ik\cdot x^1})\hat{f}(k).$$

As before we have $k_i^a \hat{f}(0)\hat{\varphi}(0) = 0$. Note

$$(\hat{\Phi}, -k_i \hat{f}\hat{\varphi}) = \int_{|k|\le 1} \frac{k_i \hat{\varphi(k)}\hat{f}(k)}{|k|^2} + \int_{|k|>1} \frac{k_i \hat{\varphi}(k)\hat{f}(k)}{|k|^2} + C \cdot 0,$$

$$|(\hat{\Phi}, -k_i \hat{f}\hat{\varphi})| \le \left| \int_{|k|\le 1} \frac{k_i \hat{\varphi(k)}\hat{f}(k)}{|k|^2} \right| + \left| \int_{|k|>1} \frac{\hat{\varphi}(k)\hat{f}(k)}{|k|^2} \right| \le I_1 + I_2,$$

where I_1, I_2 are the first and second integrals respectively. We proceed in the same manner as the proof of Lemma 7.0.3. We bound I_1 by noting

$$|I_1|^2 \le \|\hat{\varphi}\|^2_{L^2(B_1(0))} \int_{|k|\le 1} \frac{k_i^2 |(1 - e^{ik\cdot x^1})|^2 |\hat{f}(k)|^2}{|k|^4} dk$$

By Jensen's inequality we have

$$|\hat{f}|^2 = \lambda(B_r)^2 \left| \frac{1}{\lambda(B_r)} \int_{B_r} e^{-ik\cdot x} f(x)dx \right|^2 \le \lambda(B_r)^2 \frac{1}{\lambda(B_r)} \int_{B_r} |f(x)|^2 dx \le Cr^2 \|f\|_2^2,$$

and so

$$|I_1|^2 \le Cr^2 \|\hat{\varphi}\|^2_{L^2(B_1(0))} \|f\|_2^2 \int_{|k|\le 1} \frac{k_i^2 |(1 - e^{ik\cdot x^1})|^2}{|k|^4} dk.$$

We introduce the variable $z = |x|k$ to re-write the integral as

$$\int_{B_1(0)} \frac{z_i^2 |(1 - e^{iz\cdot e_x})|^2}{|z|^4} \frac{|x|^4}{|x|^2} dk = \int_{B_{|x|}(0)} \frac{z_i^2 |(1 - e^{iz\cdot e_x})|^2}{|z|^4} dz \le C + 2\pi \int_1^{|x|} \frac{1}{t^2} t dt = C + 2\pi \ln |x|.$$

The constant C is proportional to 1, since

$$\int_{B_1(0)} \frac{z_i^2 |(1 - e^{iz\cdot e_x})|^2}{|z|^4} dz \approx \int \frac{z_i^2 |1 - 1 + iz \cdot e_x|^2 + O(|z|^4)}{|z|^4} \le C\lambda(B_1(0)).$$

In fact, this integral arises when, for instance, studying the lack of crystalline order in low dimensional systems for toy models (Peierls [1979]). For small $|x|$ we use the above bound instead of the logarithm. Combining the above, we have

$$|I_1|^2 \le Cr^2 \|\varphi\|^2_{L^2(B_1(0))} \|f\|_2^2 \max\{1, \log(|x|)\},$$

To bound I_2 note that

$$\left|\int_{\mathbb{R}^2\setminus B_1(0)}\varphi(\hat{k})\frac{k_i\hat{f}(k)}{|k^2|}\right| \leq C\|\varphi\|_{L^2(\mathbb{R}^2\setminus B_1(0))}\left(\int_{\mathbb{R}^2\setminus B_1(0)}|k|^{-2}|\hat{f}(k)|^2 dk\right)^{1/2}$$
$$\leq C\|\hat{\varphi}\|_{L^2(\mathbb{R}^2\setminus B_1(0))}\|\hat{f}\|_{L^2(\mathbb{R}^2)}.$$

Combining the above by using Young's inequality and Parseval's Identity,we find that

$$|(\hat{\Phi}, -k_i\hat{f}\hat{\varphi})| \leq Cr\|\varphi\|_{L^2(\mathbb{R}^2)}\|f\|_{L^2(\mathbb{R}^2)}(1 \wedge \log|x^0|))^{1/2}.$$

This yields in particular that for all functions in $C_c^\infty(\mathbb{R}^2)$

$$|(\partial_i u, \varphi)| \leq Cr\|\varphi\|_{L^2(\mathbb{R}^2)}\|f\|_{L^2(\mathbb{R}^2)}(1 \wedge \log|x^0|))^{1/2}.$$

This implies that $u, Du \in L^2(\mathbb{R})$. $\square$

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